Higher-accuracy van der Waals density functional

Physical Review B

82,

DOI: 10.1103/physrevb.82.081101

Citation Report

#	Article	IF	Citations
1	A van der Waals density functional study of ice Ih. Journal of Chemical Physics, 2010, 133, 214503.	1.2	39
2	Power series expansion of the random phase approximation correlation energy: The role of the third- and higher-order contributions. Journal of Chemical Physics, 2010, 133, 154110.	1.2	48
3	Local response dispersion method. II. Generalized multicenter interactions. Journal of Chemical Physics, 2010, 133, 194101.	1.2	89
4	Comparative van der Waals density-functional study of graphene on metal surfaces. Physical Review B, 2010, 82, .	1.1	274
5	The Relevance of Dispersion Interactions for the Stability of Oxide Phases. Journal of Physical Chemistry C, 2010, 114, 22718-22726.	1.5	58
6	Nonlocal van der Waals density functional: The simpler the better. Journal of Chemical Physics, 2010, 133, 244103.	1.2	974
7	Secondary Structure of Ac-Ala_n-LysH⁺ Polyalanine Peptides (n =) Tj ETQq0 0 0 rgBT /Overlock 10	2.1	76
8	Adsorption of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-butane on Cu(100), Cu(111), Au(111), and Pt(111): Van der Waals density-functional study. Physical Review B, 2010, 82, .	1.1	50
9	Adsorption of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mrow><mml:mn>60</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>on Au(111) revisited: A van der Waals density functional study. Physical Review B, 2011, 83, .	1.1	53
10	Ab Initio Modeling of Donorâ€“Acceptor Interactions and Charge-Transfer Excitations in Molecular Complexes: The Case of Terthiopheneâ€“Tetracyanoquinodimethane. Journal of Chemical Theory and Computation, 2011, 7, 2068-2077.	2.3	46
11	Do Two-Dimensional â€œNoble Gas Atomsâ€•Produce Molecular Honeycombs at a Metal Surface?. Nano Letters, 2011, 11, 2944-2948.	4.5	33
12	Density Functional Theory Study of Pyrophyllite and M-Montmorillonites (M = Li, Na, K, Mg, and Ca): Role of Dispersion Interactions. Journal of Physical Chemistry A, 2011, 115, 9695-9703.	1.1	75
13	Density Functional Theory Study on Propane and Propene Adsorption on Pt(111) and PtSn Alloy Surfaces. Journal of Physical Chemistry C, 2011, 115, 9578-9586.	1.5	130
14	Adsorption of Rare-Gas Atoms and Water on Graphite and Graphene by van der Waals-Corrected Density Functional Theory. Journal of Physical Chemistry C, 2011, 115, 3695-3702.	1.5	114
15	Dispersion interactions in room-temperature ionic liquids: Results from a non-empirical density functional. Journal of Chemical Physics, 2011, 135, 154505.	1.2	18
16	Structural and Vibrational Properties of Liquid Water from van der Waals Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 3054-3061.	2.3	146
17	Ab Initio van der Waals Interactions in Simulations of Water Alter Structure from Mainly Tetrahedral to High-Density-Like. Journal of Physical Chemistry B, 2011, 115, 14149-14160.	1.2	83
18	Accurate Dispersion-Corrected Density Functionals for General Chemistry Applications. , 2011, , 1-16.		2

#	Article	IF	Citations
19	The Nature of the Binding of Au, Ag, and Pd to Benzene, Coronene, and Graphene: From Benchmark CCSD(T) Calculations to Plane-Wave DFT Calculations. Journal of Chemical Theory and Computation, 2011, 7, 3743-3755.	2.3	100
20	Doping of graphene by a Au(111) substrate: Calculation strategy within the local density approximation and a semiempirical van der Waals approach. Physical Review B, 2011, 83, .	1.1	90
21	Quantum Mechanical Modeling of Catalytic Processes. Annual Review of Chemical and Biomolecular Engineering, 2011, 2, 453-477.	3.3	68
22	Interaction of Au16 Nanocluster with Defects in Supporting Graphite: A Density-Functional Study. Journal of Physical Chemistry C, 2011, 115, 15240-15250.	1.5	23
23	GGA versus van der Waals density functional results for mixed gold/mercury molecules and pure Au and Hg cluster properties. Physical Chemistry Chemical Physics, 2011, 13, 20863.	1.3	31
24	Evaluation of Theoretical Approaches for Describing the Interaction of Water with Linear Acenes. Journal of Physical Chemistry A, 2011, 115, 5955-5964.	1.1	24
25	Real-World Predictions from Ab Initio Molecular Dynamics Simulations. Topics in Current Chemistry, 2011, 307, 109-153.	4.0	89
26	Dispersion interactions in density-functional theory: An adiabatic-connection analysis. Journal of Chemical Physics, 2011, 135, 194109.	1.2	21
27	First-principles approach to rotational-vibrational frequencies and infrared intensity for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>adsorbe in nanoporous materials. Physical Review B, 2011, 83, .	1.1	22
28	Benchmark results for empirical post-GGA functionals: Difficult exchange problems and independent tests. Physical Chemistry Chemical Physics, 2011, 13, 19325.	1.3	83
29	Comprehensive Benchmarking of a Density-Dependent Dispersion Correction. Journal of Chemical Theory and Computation, 2011, 7, 3567-3577.	2.3	400
30	Density, structure, and dynamics of water: The effect of van der Waals interactions. Journal of Chemical Physics, 2011, 134, 024516.	1.2	242
31	Entropy of Liquid Water from Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2011, 115, 14190-14195.	1.2	45
32	Performance of the van der Waals Density Functional VV10 and (hybrid)GGA Variants for Thermochemistry and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2011, 7, 3866-3871.	2.3	213
33	Comparison of the performance of dispersion-corrected density functional theory for weak hydrogen bonds. Physical Chemistry Chemical Physics, 2011, 13, 13942.	1.3	125
34	On the Importance of Gradient-Corrected Correlation for van der Waals Density Functionals. Topics in Catalysis, 2011, 54, 1143-1150.	1.3	23
35	Perspective on the structure of liquid water. Chemical Physics, 2011, 389, 1-34.	0.9	289
36	Understanding the Preferential Adsorption of CO₂ over N₂ in a Flexible Metalâ€“Organic Framework. Journal of the American Chemical Society, 2011, 133, 12849-12857.	6.6	103

#	Article	IF	Citations
37	van der Waals interaction between an atom and a spherical plasma shell. Physical Review B, 2011, 83, .	1.1	6
38	Van der Waals density functionals applied to solids. Physical Review B, 2011, 83, .	1.1	3,608
39	Dispersion Interactions with Density-Functional Theory: Benchmarking Semiempirical and Interatomic Pairwise Corrected Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 3944-3951.	2.3	265
40	Density functional theory with London dispersion corrections. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 211-228.	6.2	2,030
41	noloco: An efficient implementation of van der Waals density functionals based on a Monte-Carlo integration technique. Computer Physics Communications, 2011, 182, 1657-1662.	3.0	20
42	Benchmarking Density Functional Methods against the S66 and S66x8 Datasets for Nonâ€Covalent Interactions. ChemPhysChem, 2011, 12, 3421-3433.	1.0	283
43	Van der Waals density functional calculations of binding in molecular crystals. Computer Physics Communications, 2011, 182, 1800-1804.	3.0	44
44	Vanadium pentoxide (V2O5): A van der Waals density functional study. Computer Physics Communications, 2011, 182, 1805-1809.	3.0	44
45	Structural and zero-point vibrational effects on the electric dipole moments and static dipole polarizabilities of sodium clusters. Physical Review B, 2011, 84, .	1.1	23
46	Evaluation of a density functional with account of van der Waals forces using experimental data of H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>physisorption on Cu(111). Physical Review B, 2011, 84, .	1.1	46
47	Adsorption of Alq<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>on Mg(001) surface: Role of chemical bonding, molecular distortion, and van der Waals interaction. Physical Review B, 2011, 83, .	1.1	7
48	Graphene nanogap for gate-tunable quantum-coherent single-molecule electronics. Physical Review B, 2011, 84, .	1.1	25
49	Ab initioenergetics and kinetics study of H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>and CH<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>in the SI clathrate hydrate. Physical Review B, 2011, 84, .	1.1	30
50	Van der Waals density functional study of energetic, structural, and vibrational properties of small water clusters and ice<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>I</mml:mi><mml:mrow><mml:mi>h</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review B, 2011, 84, .	1.1	46
51	Noble gases on metal surfaces: Insights on adsorption site preference. Physical Review B, 2011, 84, .	1.1	33
52	Pseudopotential approximation in van der Waals density functional calculations. Physical Review B, 2011, 84, .	1.1	20
53	Self-assembled cyclic oligothiophene nanotubes: Electronic properties from a dispersion-corrected hybrid functional. Physical Review B, 2011, 84, .	1.1	30
54	Stabilizing Graphitic Thin Films of Wurtzite Materials by Epitaxial Strain. Physical Review Letters, 2011, 107, 236101.	2.9	88

#	Article	IF	Citations
55	Stacking and band structure of van der Waals bonded graphane multilayers. Physical Review B, 2011, 83, .	1.1	44
56	Pt on graphene monolayers supported on a Ni(111) substrate: Relativistic density-functional calculations. Journal of Chemical Physics, 2012, 136, 074701.	1.2	17
57	Atomic volumes and polarizabilities in density-functional theory. Journal of Chemical Physics, 2012, 136, 034109.	1.2	29
58	Water monomer interaction with gold nanoclusters from van der Waals density functional theory. Journal of Chemical Physics, 2012, 136, 024702.	1.2	15
59	Helium mediated deposition: Modeling the Heâ"TiO₂(110)-(1Ã—1) interaction potential and application to the collision of a helium droplet from density functional calculations. Journal of Chemical Physics, 2012, 136, 124703.	1.2	31
60	Effect of dispersion correction on the Au(1 1 1)-H2O interface: A first-principles study. Journal of Chemical Physics, 2012, 137, 114709.	1.2	49
61	Structural, elastic, and vibrational properties of layered titanium dichalcogenides: A van der Waals density functional study. Journal of Chemical Physics, 2012, 137, 224509.	1.2	19
62	Assessment of dispersion corrections in DFT calculations on large biological systems. Molecular Physics, 2012, 110, 3061-3076.	0.8	8
63	Analyzing the frequency shift of physiadsorbed CO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>in metal organic framework materials. Physical Review B, 2012, 85, .	1.1	46
64	Adsorption of tris(8-hydroxyquinoline)aluminum molecules on cobalt surfaces. Physical Review B, 2012, 85, .	1.1	19
65	Origin of nanomechanical motion in a single-C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>60</mml:mn></mml:msub></mml:math>transistor. Physical Review B, 2012, 85, .	1.1	4
66	Response of the Shockley surface state to an external electrical field: A density-functional theory study of Cu(111). Physical Review B, 2012, 85, .	1.1	19
67	Structure and energetics of a ferroelectric organic crystal of phenazine and chloranilic acid. Physical Review B, 2012, 86, .	1.1	24
68	Accurate and Efficient Method for Many-Body van der Waals Interactions. Physical Review Letters, 2012, 108, 236402.	2.9	1,120
69	Nonequilibrium thermodynamics of interacting tunneling transport: variational grand potential, density functional formulation and nature of steady-state forces. Journal of Physics Condensed Matter, 2012, 24, 424219.	0.7	14
70	Insights into the structure and dynamics of liquid water: A comparative study of conventional QM/MM and ONIOM-XS MD simulations. Journal of Molecular Liquids, 2012, 174, 26-33.	2.3	13
71	Ab Initio Calculations of the Interaction between CO₂ and the Acetate Ion. Journal of Physical Chemistry A, 2012, 116, 11643-11650.	1.1	50
72	CO2 Capture by Metalâ€"Organic Frameworks with van der Waals Density Functionals. Journal of Physical Chemistry A, 2012, 116, 4957-4964.	1.1	92

#	Article	IF	Citations
73	The properties of hydrogen and helium under extreme conditions. Reviews of Modern Physics, 2012, 84, 1607-1653.	16.4	425
74	Performance of dispersion-corrected density functional theory for the interactions in ionic liquids. Physical Chemistry Chemical Physics, 2012, 14, 4875.	1.3	202
75	Van der Waals forces in the perfluorinated metalâ€“organic framework zinc 1,2-bis(4-pyridyl)ethane tetrafluoroterephthalate. Physical Chemistry Chemical Physics, 2012, 14, 7059.	1.3	20
76	Random-phase approximation and its applications in computational chemistry and materials science. Journal of Materials Science, 2012, 47, 7447-7471.	1.7	479
77	van der Waals Interaction Energies of Small Fragments of P, As, Sb, S, Se, and Te: Comparison of Complete Basis Set Limit CCSD(T) and DFT with Approximate Dispersion. Journal of Chemical Theory and Computation, 2012, 8, 2301-2309.	2.3	6
78	Ab initioinvestigation of the electronic properties of graphene on InAs(111)A. Journal of Physics Condensed Matter, 2012, 24, 485004.	0.7	3
79	A first-principles-based correlation functional for harmonious connection of short-range correlation and long-range dispersion. Journal of Chemical Physics, 2012, 137, 204121.	1.2	6
80	Dispersion Interactions and Vibrational Effects in Ice as a Function of Pressure: A First Principles Study. Physical Review Letters, 2012, 108, 105502.	2.9	55
81	Elastic and Vibrational Properties of Î±- and Î²-PbO.. Journal of Physical Chemistry C, 2012, 116, 21514-21522.	1.5	38
82	Spherical-shell model for the van der Waals coefficients between fullerenes and/or nearly spherical nanoclusters. Journal of Physics Condensed Matter, 2012, 24, 424207.	0.7	12
83	Van der Waals Coefficients for Nanostructures: Fullerenes Defy Conventional Wisdom. Physical Review Letters, 2012, 109, 233203.	2.9	66
84	Modeling van der Waals Interactions in Zeolites with Periodic DFT: Physisorption of n-Alkanes in ZSM-22. Catalysis Letters, 2012, 142, 1057-1060.	1.4	61
85	Prediction of CO₂ Adsorption Properties in Zeolites Using Force Fields Derived from Periodic Dispersion-Corrected DFT Calculations. Journal of Physical Chemistry C, 2012, 116, 10692-10701.	1.5	123
86	First-principles theoretical study of organic/metal interfaces: Vacuum level shifts and interface dipoles. Current Applied Physics, 2012, 12, S2-S9.	1.1	18
87	Electrochemical properties of crystallized dilithium squarate: insight from dispersion-corrected density functional theory. Physical Chemistry Chemical Physics, 2012, 14, 11398.	1.3	23
88	Structural and vibrational properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-MoO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>from van der Waals corrected density functional theory calculations. Physical Review B, 2012, 85, .	1.1	47
89	Insight into the Adsorption of Water on the Clean CeO₂(111) Surface with van der Waals and Hybrid Density Functionals. Journal of Physical Chemistry C, 2012, 116, 13584-13593.	1.5	116
90	Short range DFT combined with long-range local RPA within a range-separated hybrid DFT framework. Chemical Physics Letters, 2012, 550, 162-169.	1.2	29

#	Article	IF	Citations
91	Ligand-Assisted Enhancement of CO₂ Capture in Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2012, 134, 6714-6719.	6.6	95
92	Chemical Transformations Drive Complex Self-Assembly of Uracil on Close-Packed Coinage Metal Surfaces. ACS Nano, 2012, 6, 2477-2486.	7.3	55
93	Adsorption of rare-gas atoms on Cu(111) and Pb(111) surfaces by van der Waals corrected density functional theory. Physical Review B, 2012, 85, .	1.1	47
94	A benchmark for non-covalent interactions in solids. Journal of Chemical Physics, 2012, 137, 054103.	1.2	300
95	Physisorption of nucleobases on graphene: a comparative van der Waals study. Journal of Physics Condensed Matter, 2012, 24, 424210.	0.7	83
96	Ab initiostudies of hydrogen adatoms on bilayer graphene. Physical Review B, 2012, 85, .	1.1	64
97	Density functionals for surface science: Exchange-correlation model development with Bayesian error estimation. Physical Review B, 2012, 85, .	1.1	1,087
98	A Density Functional Theory Study of Cytosine on Au(111). Journal of Physical Chemistry C, 2012, 116, 21366-21373.	1.5	38
99	Nanostructured Diamineâ€“Fullerene Derivatives: Computational Density Functional Theory Study and Experimental Evidence for their Formation via Gas-Phase Functionalization. Journal of Physical Chemistry A, 2012, 116, 1663-1676.	1.1	15
100	Ab initio carbon capture in open-site metalâ€“organic frameworks. Nature Chemistry, 2012, 4, 810-816.	6.6	310
101	Graphene on metal surfaces and its hydrogen adsorption: A meta-GGA functional study. Physical Review B, 2012, 86, .	1.1	57
102	Constrained Density Functional Theory. Chemical Reviews, 2012, 112, 321-370.	23.0	454
103	State-of-the-art and challenges in theoretical simulations of heterogeneous catalysis at the microscopic level. Catalysis Science and Technology, 2012, 2, 2405.	2.1	38
104	Electronic properties and STM images of doped bilayer graphene. Physical Review B, 2012, 85, .	1.1	30
105	Towards chemically accurate simulation of moleculeâ€“surface reactions. Physical Chemistry Chemical Physics, 2012, 14, 14966.	1.3	80
106	First-Principles Calculations of Propane Dehydrogenation over PtSn Catalysts. ACS Catalysis, 2012, 2, 1247-1258.	5.5	235
107	Assessment of ten DFT methods in predicting structures of sheet silicates: Importance of dispersion corrections. Journal of Chemical Physics, 2012, 137, 114105.	1.2	117
108	DFT simulation of vibrational properties of adenine adsorbed on gold surface: The effect of periodic boundary conditions. Computational and Theoretical Chemistry, 2012, 993, 106-112.	1.1	10

#	Article	IF	Citations
109	Perspective: Advances and challenges in treating van der Waals dispersion forces in density functional theory. Journal of Chemical Physics, 2012, 137, 120901.	1.2	931
110	Adsorption of water on graphene: A van der Waals density functional study. Physical Review B, 2012, 86, .	1.1	88
111	Benchmark Assessment of the Accuracy of Several van der Waals Density Functionals. Journal of Chemical Theory and Computation, 2012, 8, 1929-1934.	2.3	93
112	van der Waals density functional study of CO2binding in zeolitic imidazolate frameworks. Physical Review B, 2012, 85, .	1.1	22
114	Molecular adsorption on metal surfaces with van der Waals density functionals. Physical Review B, 2012, 85, .	1.1	89
115	Ab initioand semi-empirical van der Waals study of grapheneâ€“boron nitride interaction from a molecular point of view. Journal of Physics Condensed Matter, 2012, 24, 424214.	0.7	26
116	Improved description of soft layered materials with van der Waals density functional theory. Journal of Physics Condensed Matter, 2012, 24, 424216.	0.7	150
117	van der Waals density functional for solids. Physical Review B, 2012, 86, .	1.1	74
118	Are we van der Waals ready?. Journal of Physics Condensed Matter, 2012, 24, 424218.	0.7	129
119	Fluctuations in ambient water. Journal of Molecular Liquids, 2012, 176, 2-16.	2.3	86
120	The role of van der Waals interactions in the adsorption of noble gases on metal surfaces. Journal of Physics Condensed Matter, 2012, 24, 424211.	0.7	42
121	Global Minima of Protonated Water Clusters (H₂O)₂₀H⁺ Revisited. Journal of Physical Chemistry A, 2012, 116, 10826-10835.	1.1	14
122	Tungsten Oxide Clathrates for Water Oxidation: A First Principles Study. Chemistry of Materials, 2012, 24, 4252-4260.	3.2	37
123	Benchmarking van der Waals density functionals with experimental data: potential-energy curves for H₂molecules on Cu(111), (100) and (110) surfaces. Journal of Physics Condensed Matter, 2012, 24, 424213.	0.7	35
124	Reliable DFT-based estimates of cohesive energies of organic solids: The anthracene crystal. Journal of Chemical Physics, 2012, 137, 194311.	1.2	12
125	Assessing the importance of Van der Waals interactions on the adsorption of azobenzene on the rutile TiO2(110) surface. Chemical Physics Letters, 2012, 545, 60-65.	1.2	13
126	Ab initio study of energy-band modulation in graphene-based two-dimensional layered superlattices. Journal of Materials Chemistry, 2012, 22, 23821.	6.7	18
127	Ab Initio Parametrized Force Field for the Flexible Metalâ€“Organic Framework MIL-53(Al). Journal of Chemical Theory and Computation, 2012, 8, 3217-3231.	2.3	69

#	Article	IF	Citations
128	Benzene adsorbed on metals: Concerted effect of covalency and van der Waals bonding. Physical Review B, 2012, 86, .	1.1	243
129	MOLECULAR BIOLOGY AT THE QUANTUM LEVEL: CAN MODERN DENSITY FUNCTIONAL THEORY FORGE THE PATH?. Nano LIFE, 2012, 02, 1230006.	0.6	8
130	A Hierarchy of Methods for the Energetically Accurate Modeling of Isomerism in Monosaccharides. Journal of Chemical Theory and Computation, 2012, 8, 2630-2645.	2.3	52
131	Rationale for switching to nonlocal functionals in density functional theory. Journal of Physics Condensed Matter, 2012, 24, 424215.	0.7	18
132	Noncovalent Interactions in SIESTA Using the vdW-DF Functional: S22 Benchmark and Macrocyclic Structures. Journal of Chemical Theory and Computation, 2012, 8, 281-289.	2.3	26
133	Ab initio derived forceâ€field parameters for molecular dynamics simulations of deprotonated amorphousâ€SiO₂/water interfaces. Physica Status Solidi (B): Basic Research, 2012, 249, 292-305.	0.7	71
134	Symmetryâ€adapted perturbation theory of intermolecular forces. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 254-272.	6.2	478
135	mathcal{O}(N) methods in electronic structure calculations. Reports on Progress in Physics, 2012, 75, 036503.	8.1	432
136	Challenges for Density Functional Theory. Chemical Reviews, 2012, 112, 289-320.	23.0	1,869
137	Calculation of dispersion energies. Journal of Physics Condensed Matter, 2012, 24, 073201.	0.7	187
138	Dispersion-Corrected Density Functional Theory and Classical Force Field Calculations of Water Loading on a Pyrophyllite(001) Surface. Journal of Physical Chemistry C, 2012, 116, 17134-17141.	1.5	40
139	A simplified implementation of van der Waals density functionals for first-principles molecular dynamics applications. Journal of Chemical Physics, 2012, 136, 224107.	1.2	49
140	van der Waals Bonding in Layered Compounds from Advanced Density-Functional First-Principles Calculations. Physical Review Letters, 2012, 108, 235502.	2.9	851
141	Comparing van der Waals Density Functionals for CO₂ Adsorption in Metal Organic Frameworks. Journal of Physical Chemistry C, 2012, 116, 16957-16968.	1.5	72
142	On the Adsorption of Formaldehyde and Methanol on a Water-Covered Pt(111): a DFT-D Study. Journal of Physical Chemistry C, 2012, 116, 15484-15492.	1.5	37
143	Twoâ€Dimensional Nanostructured Growth of Nanoclusters and Molecules on Insulating Surfaces. Advanced Materials, 2012, 24, 3228-3232.	11.1	22
144	van der Waals interaction in magnetic bilayer graphene nanoribbons. Physical Review B, 2012, 85, .	1.1	41
145	Water wetting on representative metal surfaces: Improved description from van der Waals density functionals. Chemical Physics Letters, 2012, 521, 161-166.	1.2	18

#	Article	IF	Citations
146	Performance of dispersion-corrected density functional theory for thermochemistry and non-covalent interactions. Journal of Cheminformatics, 2012, 4, .	2.8	4
147	Aromatic Interactions as Control Elements in Stereoselective Organic Reactions. Accounts of Chemical Research, 2013, 46, 979-989.	7.6	216
148	A novel correction scheme for DFT: A combined vdW-DF/CCSD(T) approach. Journal of Chemical Physics, 2013, 139, 034115.	1.2	18
149	Mechanical properties of hydrogenated bilayer graphene. Journal of Chemical Physics, 2013, 138, 244709.	1.2	4
150	Van der Waals density-functional study of 100% hydrogen coverage on bilayer graphene. Computational Materials Science, 2013, 78, 1-8.	1.4	1
151	Stepwise self-assembly of C60 mediated by atomic scale moirÃ© magnifiers. Nature Communications, 2013, 4, 1679.	5.8	31
152	Van der Waals interactions in density functional theory by combining the quantum harmonic oscillator-model with localized Wannier functions. Journal of Chemical Physics, 2013, 139, 054106.	1.2	34
153	GolP-CHARMM: First-Principles Based Force Fields for the Interaction of Proteins with Au(111) and Au(100). Journal of Chemical Theory and Computation, 2013, 9, 1616-1630.	2.3	210
154	Nonlocal van der Waals Approach Merged with Double-Hybrid Density Functionals: Toward the Accurate Treatment of Noncovalent Interactions. Journal of Chemical Theory and Computation, 2013, 9, 3437-3443.	2.3	53
155	Understanding the role of vibrations, exact exchange, and many-body van der Waals interactions in the cohesive properties of molecular crystals. Journal of Chemical Physics, 2013, 139, 024705.	1.2	260
156	Origins of CH₄/CO₂ Adsorption Selectivity in Zeolitic Imidazolate Frameworks: A van der Waals Density Functional Study. Journal of Physical Chemistry C, 2013, 117, 14642-14651.	1.5	16
157	Cl-intercalated graphene on SiC: Influence of van der Waals forces. Europhysics Letters, 2013, 101, 27008.	0.7	11
158	Peculiar diffusion of C60 on In-adsorbed Si(111)â^š3 Ã— â^š3-Au surface. Surface Science, 2013, 616, 44-50.	0.8	12
159	Theoretical assessment of graphene-metal contacts. Journal of Chemical Physics, 2013, 138, 244701.	1.2	58
160	Assessment of Coupled Cluster Theory and more Approximate Methods for Hydrogen Bonded Systems. Journal of Chemical Theory and Computation, 2013, 9, 4403-4413.	2.3	41
161	Free Energies of Binding from Large-Scale First-Principles Quantum Mechanical Calculations: Application to Ligand Hydration Energies. Journal of Physical Chemistry B, 2013, 117, 9478-9485.	1.2	41
162	Coverage-Dependent Interactions at the Organicsâ€“Metal Interface: Quinonoid Zwitterions on Au(111). Journal of Physical Chemistry C, 2013, 117, 16406-16415.	1.5	21
163	How Theoretical Simulations Can Address the Structure and Activity of Nanoparticles. Topics in Catalysis, 2013, 56, 1262-1272.	1.3	16

#	Article	IF	Citations
164	An improved treatment of empirical dispersion and a many-body energy decomposition scheme for the explicit polarization plus symmetry-adapted perturbation theory (XSAPT) method. Journal of Chemical Physics, 2013, 139, 034107.	1.2	60
165	Spinâ€componentâ€scaled double hybrids: An extensive search for the best fifthâ€rung functionals blending DFT and perturbation theory. Journal of Computational Chemistry, 2013, 34, 2327-2344.	1.5	292
166	Contribution of van der Waals interactions to the adsorption energy of C2H2, C2H4, and C6H6 on Si(100). Chemical Physics Letters, 2013, 557, 159-162.	1.2	11
167	The PYXAID Program for Non-Adiabatic Molecular Dynamics in Condensed Matter Systems. Journal of Chemical Theory and Computation, 2013, 9, 4959-4972.	2.3	588
168	Evaluating London Dispersion Force Corrections in Crystalline Nitroguanidine by Terahertz Spectroscopy. IEEE Transactions on Terahertz Science and Technology, 2013, 3, 281-287.	2.0	22
169	Structure and stability of acrolein and allyl alcohol networks on Ag(111) from density functional theory based calculations with dispersion corrections. Surface Science, 2013, 617, 175-182.	0.8	6
170	Study of ligand effects in aurophilic interactions using local correlation methods. Physical Chemistry Chemical Physics, 2013, 15, 18115.	1.3	37
171	Improving the Adsorption of Au Atoms and Nanoparticles on Graphite via Li Intercalation. Journal of Physical Chemistry C, 2013, 117, 22683-22695.	1.5	4
172	Ab initio study of electronic and optical behavior of two-dimensional silicon carbide. Journal of Materials Chemistry C, 2013, 1, 2131.	2.7	148
173	Deliquescence of NaBH4 from Density Functional Theory and Experiments. Industrial & Engineering Chemistry Research, 2013, 52, 13849-13861.	1.8	4
174	Terahertz Vibrations of Crystalline Acyclic and Cyclic Diglycine: Benchmarks for London Force Correction Models. Journal of Physical Chemistry A, 2013, 117, 10504-10512.	1.1	19
175	Thermodynamic Equilibrium Conditions of Graphene Films on SiC. Physical Review Letters, 2013, 111, 065502.	2.9	34
176	Quantum Monte Carlo applied to solids. Physical Review B, 2013, 88, .	1.1	81
177	Critical Importance of van der Waals Stabilization in Strongly Chemically Bonded Surfaces: Cu(110):O. Journal of Chemical Theory and Computation, 2013, 9, 5578-5584.	2.3	10
178	Structural and electronic properties of perylene from first principles calculations. Journal of Chemical Physics, 2013, 138, 094509.	1.2	35
179	Structures, Energetics, and Electronic Properties of Layered Materials and Nanotubes of Cadmium Chalcogenides. Journal of Physical Chemistry C, 2013, 117, 25817-25825.	1.5	26
180	Room temperature compressibility and diffusivity of liquid water from first principles. Journal of Chemical Physics, 2013, 139, 194502.	1.2	54
181	Theoretical study of solid iron nanocrystal movement inside a carbon nanotube. Physical Review B, 2013, 88, .	1.1	2

#	Article	IF	Citations
182	Accurate non-covalent interactions with basis-set corrections from interference-corrected perturbation theory: comparison with the S22B database. Molecular Physics, 2013, 111, 2299-2305.	0.8	15
183	Effect of van der Waals interactions on H2 dissociation on clean and defected Ru(0001) surface. European Physical Journal B, 2013, 86, 1.	0.6	6
184	Molecular Heterogeneity of Polystyrene-Modified Fullerene Core Stars. Macromolecules, 2013, 46, 7451-7457.	2.2	3
185	Trends in Adsorption Characteristics of Benzene on Transition Metal Surfaces: Role of Surface Chemistry and van der Waals Interactions. Journal of Physical Chemistry C, 2013, 117, 20572-20583.	1.5	147
186	Interatomic methods for the dispersion energy derived from the adiabatic connection fluctuation-dissipation theorem. Journal of Chemical Physics, 2013, 138, 074106.	1.2	129
187	Volume shrinkage of a metalâ€“organic framework host induced by the dispersive attraction of guest gas molecules. Physical Chemistry Chemical Physics, 2013, 15, 18822.	1.3	23
188	First principles derived, transferable force fields for CO2 adsorption in Na-exchanged cationic zeolites. Physical Chemistry Chemical Physics, 2013, 15, 12882.	1.3	79
189	Electronic properties of graphene on the C-decorated Si(111) surface: An ab initio study. Current Applied Physics, 2013, 13, 1512-1519.	1.1	2
190	Quantum Chemical Challenges for the Binding of Simple Alkanes to Supramolecular Hosts. Journal of Physical Chemistry B, 2013, 117, 13409-13417.	1.2	24
191	Rhodizonic Acid on Noble Metals: Surface Reactivity and Coordination Chemistry. Journal of Physical Chemistry Letters, 2013, 4, 3413-3419.	2.1	14
192	A transferable H2O interaction potential based on a single center multipole expansion: SCME. Physical Chemistry Chemical Physics, 2013, 15, 16542.	1.3	32
193	Dispersion Corrected Hartreeâ€“Fock and Density Functional Theory for Organic Crystal Structure Prediction. Topics in Current Chemistry, 2013, 345, 1-23.	4.0	72
194	Communication: Analytic gradients in the random-phase approximation. Journal of Chemical Physics, 2013, 139, 081101.	1.2	38
195	Effects of atomic scale roughness at metal/insulator interfaces on metal work function. Physical Chemistry Chemical Physics, 2013, 15, 19615.	1.3	19
196	Assessment of Kohnâ€“Sham density functional theory and MÃ¸llerâ€“Plesset perturbation theory for ionic liquids. Physical Chemistry Chemical Physics, 2013, 15, 13664.	1.3	98
197	Thermodynamic screening of metal-substituted MOFs for carbon capture. Physical Chemistry Chemical Physics, 2013, 15, 4573.	1.3	62
198	Interplay between Hydrogen Bonding and Moleculeâ€“Substrate Interactions in the Case of Terephthalic Acid Molecules on Cu(001) Surfaces. Journal of Physical Chemistry C, 2013, 117, 1287-1296.	1.5	36
199	Ab initio optical study of graphene on hexagonal boron nitride and fluorographene substrates. Journal of Materials Chemistry C, 2013, 1, 1618.	2.7	39

#	Article	IF	Citations
200	The role of van der Waals forces in water adsorption on metals. Journal of Chemical Physics, 2013, 138, 024708.	1.2	173
201	A Critical Assessment of Two-Body and Three-Body Interactions in Water. Journal of Chemical Theory and Computation, 2013, 9, 1103-1114.	2.3	126
202	Ab initio molecular dynamics study of the Helmholtz layer formed on solidâ€“liquid interfaces and its capacitance. Chemical Physics Letters, 2013, 556, 9-12.	1.2	27
203	HOMO band dispersion of crystalline rubrene: Effects of self-energy corrections within theGWapproximation. Physical Review B, 2013, 88, .	1.1	38
204	(H₂O)₂₀ Water Clusters at Finite Temperatures. Journal of Physical Chemistry A, 2013, 117, 9985-9998.	1.1	19
205	Ï€-Stacked polyphenolic dimers: A case study using dispersion-corrected methods. Chemical Physics Letters, 2013, 578, 120-125.	1.2	11
206	Effects of van der Waals interaction for first-principles calculations on iron-based superconductors. Physica C: Superconductivity and Its Applications, 2013, 494, 9-12.	0.6	3
207	Theoretical investigation of layered zeolite frameworks: Interaction between IPC-1P layers derived from zeolite UTL. Catalysis Today, 2013, 204, 15-21.	2.2	33
208	Noncovalent Interactions of DNA Bases with Naphthalene and Graphene. Journal of Chemical Theory and Computation, 2013, 9, 2090-2096.	2.3	73
209	Chiral â€œPinwheelâ€•Heterojunctions Self-Assembled from C₆₀ and Pentacene. ACS Nano, 2013, 7, 3086-3094.	7.3	16
210	Catalysis by Doped Oxides. Chemical Reviews, 2013, 113, 4391-4427.	23.0	687
211	Nuclear Quantum Effects and Nonlocal Exchange-Correlation Functionals Applied to Liquid Hydrogen at High Pressure. Physical Review Letters, 2013, 110, 065702.	2.9	150
212	Is there a Difference in Van Der Waals Interactions between Rare Gas Atoms Adsorbed on Metallic and Semiconducting Single-Walled Carbon Nanotubes?. Physical Review Letters, 2013, 110, 135503.	2.9	19
214	Performance of Non-Local and Atom-Pairwise Dispersion Corrections to DFT for Structural Parameters of Molecules with Noncovalent Interactions. Journal of Chemical Theory and Computation, 2013, 9, 308-315.	2.3	91
215	Density Functional Theoretical Study of Graphene on Transition-Metal Surfaces: The Role of Metal d-Band in the Potential-Energy Surface. Journal of Physical Chemistry C, 2013, 117, 8156-8160.	1.5	19
216	Adsorption capacity of H2O, NH3, CO, and NO2 on the pristine graphene. Journal of Applied Physics, 2013, 113, .	1.1	80
217	Theoretical study on the interaction between graphene divacancies and C2H2. Chemical Physics Letters, 2013, 567, 43-47.	1.2	3
218	What Can We Learn about Dispersion from the Conformer Surface of n-Pentane?. Journal of Physical Chemistry A, 2013, 117, 3118-3132.	1.1	60

#	Article	IF	Citations
219	Tkatchenko-Scheffler van der Waals correction method with and without self-consistent screening applied to solids. Physical Review B, 2013, 87, .	1.1	293
220	Effect of van der Waals Interactions on the Adsorption of Olympicene Radical on Cu(111): Characteristics of Weak Physisorption versus Strong Chemisorption. Journal of Physical Chemistry C, 2013, 117, 2893-2902.	1.5	52
221	Surface Atom Motion to Move Iron Nanocrystals through Constrictions in Carbon Nanotubes under the Action of an Electric Current. Physical Review Letters, 2013, 110, 185901.	2.9	18
222	Optical properties of tungsten trioxide from first-principles calculations. Physical Review B, 2013, 87, .	1.1	71
223	Accounting for van der Waals interactions between adsorbates and surfaces in density functional theory based calculations: selected examples. RSC Advances, 2013, 3, 13085.	1.7	138
224	Towards a predictive first-principles description of solid molecular hydrogen with density functional theory. Physical Review B, 2013, 87, .	1.1	75
225	Experimental and Theoretical Comparison of Gas Desorption Energies on Metallic and Semiconducting Single-Walled Carbon Nanotubes. Journal of the American Chemical Society, 2013, 135, 7768-7776.	6.6	20
226	Gate-Tunable Large Negative Tunnel Magnetoresistance in Niâ€“C₆₀â€“Ni Single Molecule Transistors. Nano Letters, 2013, 13, 481-485.	4.5	86
227	Computational modelling of inorganic solids. Annual Reports on the Progress of Chemistry Section A, 2013, 109, 421.	0.8	3
228	Initial Growth of N,Nâ€²-Bis(1-ethylpropyl)perylene-3,4,9,10-tetracarboxdiimide Films on Cu(100). Journal of Physical Chemistry C, 2013, 117, 11679-11685.	1.5	7
229	Nonlocal van der Waals functionals: The case of rare-gas dimers and solids. Journal of Chemical Physics, 2013, 138, 204103.	1.2	42
230	Non-covalent interactions and thermochemistry using XDM-corrected hybrid and range-separated hybrid density functionals. Journal of Chemical Physics, 2013, 138, 204109.	1.2	130
231	A family of zeolites with controlled pore size prepared using a top-down method. Nature Chemistry, 2013, 5, 628-633.	6.6	355
232	Interaction between Coronene and Graphite from Temperature-Programmed Desorption and DFT-vdW Calculations: Importance of Entropic Effects and Insights into Graphite Interlayer Binding. Journal of Physical Chemistry C, 2013, 117, 13520-13529.	1.5	45
233	Quantum mechanical treatment of binding energy between DNA nucleobases and carbon nanotube: A DFT analysis. Physica E: Low-Dimensional Systems and Nanostructures, 2013, 54, 65-71.	1.3	20
234	van der Waals bonding and the quasiparticle band structure of SnO from first principles. Physical Review B, 2013, 87, .	1.1	55
235	Structural, elastic and electronic properties of GaSe under biaxial and uniaxial compressive stress. Journal of Physics and Chemistry of Solids, 2013, 74, 1240-1248.	1.9	27
236	Linear Compressibility and Thermal Expansion of KMn[Ag(CN)₂]₃ Studied by Raman Spectroscopy and First-Principles Calculations. Journal of Physical Chemistry C, 2013, 117, 25704-25713.	1.5	18

#	Article	IF	Citations
237	van der Waals-Corrected Ab Initio Study of Water Iceâ€“Graphite Interaction. Journal of Physical Chemistry C, 2013, 117, 321-325.	1.5	26
238	Controlling Carboxyl Deprotonation on Cu(001) by Surface Sn Alloying. Journal of Physical Chemistry C, 2013, 117, 17058-17065.	1.5	16
239	Hierarchical simulations of hybrid polymerâ€“solid materials. Soft Matter, 2013, 9, 6696.	1.2	61
240	Interlayer interactions in graphites. Scientific Reports, 2013, 3, 3046.	1.6	171
241	Influence of spin-phonon coupling on antiferromagnetic spin fluctuations in FeSe under pressure: First-principles calculations with van der Waals corrections. Physical Review B, 2013, 88, .	1.1	23
242	5-Methylation of Cytosine in CG:CG Base-Pair Steps: A Physicochemical Mechanism for the Epigenetic Control of DNA Nanomechanics. Journal of Physical Chemistry B, 2013, 117, 16436-16442.	1.2	22
243	Probing Adsorption Interactions in Metalâ€“Organic Frameworks using X-ray Spectroscopy. Journal of the American Chemical Society, 2013, 135, 18183-18190.	6.6	56
244	DFT Studies of Pristine Hexagonal Ge₁Sb₂Te₄(0001), Ge₂Sb₂Te₅(0001), and Ge₁Sb₄Te₇(0001) Surfaces. Journal of Physical Chemistry C, 2013, 117, 15075-15089.	1.5	29
245	Analysis of van der Waals density functional components: Binding and corrugation of benzene and C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>60</mml:mn></mml:msub></mml:math>on boron nitride and graphene. Physical Review B, 2013, 87, .	1.1	95
246	Appropriate description of intermolecular interactions in the methane hydrates: An assessment of DFT methods. Journal of Computational Chemistry, 2013, 34, 121-131.	1.5	111
247	AA stacking, tribological and electronic properties of double-layer graphene with krypton spacer. Journal of Chemical Physics, 2013, 139, 154705.	1.2	23
248	N-density representability and the optimal transport limit of the Hohenberg-Kohn functional. Journal of Chemical Physics, 2013, 139, 164109.	1.2	26
249	Structure and energetics of benzene adsorbed on transition-metal surfaces: density-functional theory with van der Waals interactions including collective substrate response. New Journal of Physics, 2013, 15, 053046.	1.2	143
250	Non-additivity of polarizabilities and van der Waals C6 coefficients of fullerenes. Journal of Chemical Physics, 2013, 138, 114107.	1.2	34
251	Interactions between stacked layers of phenyl-modified silicene. New Journal of Physics, 2013, 15, 125018.	1.2	13
252	The quantum nature of the OH stretching mode in ice and water probed by neutron scattering experiments. Journal of Chemical Physics, 2013, 139, 074504.	1.2	39
253	Electron-doped organics: Charge-disproportionate insulators and Hubbard-FrÃ¶hlich metals. Physical Review B, 2013, 88, .	1.1	16
254	Intermolecular interactions and substrate effects for an adamantane monolayer on a Au(111) surface. Physical Review B, 2013, 88, .	1.1	6

#	Article	IF	Citations
255	Harris-type van der Waals density functional scheme. Physical Review B, 2013, 88, .	1.1	8
256	Nonlocal van der Waals density functional made simple and efficient. Physical Review B, 2013, 87, .	1.1	471
257	Quasiparticle spectra and excitons of organic molecules deposited on substrates:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msub></mml:mrow></mml:math> approach applied to benzene on graphene and metallic substrates. Physical Review B, 2013, 88, .	1.1	19
258	Inclusion of screening effects in the van der Waals corrected DFT simulation of adsorption processes on metal surfaces. Physical Review B, 2013, 87, .	1.1	22
259	Thermodynamic stability of alkali-metalâ€“zinc double-cation borohydrides at low temperatures. Physical Review B, 2013, 88, .	1.1	29
260	Quantification of finite-temperature effects on adsorption geometries of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ï€</mml:mi></mml:math>-conjugated molecules: Azobenzene/Ag(111). Physical Review B, 2013, 88, .	1.1	43
261	Label-free molecular detection with capped carbon nanotubes. Applied Physics Letters, 2013, 102, 083103.	1.5	1
262	Efficient basis sets for non-covalent interactions in XDM-corrected density-functional theory. Journal of Chemical Physics, 2013, 139, 214109.	1.2	29
263	On the accuracy of van der Waals inclusive density-functional theory exchange-correlation functionals for ice at ambient and high pressures. Journal of Chemical Physics, 2013, 139, 154702.	1.2	119
264	Structure and functionality of bromine doped graphite. Journal of Chemical Physics, 2013, 138, 164702.	1.2	8
265	Interaction of Platinum Nanoparticles with Graphitic Carbon Structures: A Computational Study. ChemPhysChem, 2013, 14, 2984-2989.	1.0	36
266	Intramolecular Hydroalkoxylation of Nonâ€Activated Cï£¾C Bonds Catalysed by Zeolites: An Experimental and Theoretical Study. ChemSusChem, 2013, 6, 1021-1030.	3.6	10
267	Implementation of van der Waals Density Functional Approach to the Spin-Polarized System: Interaction Potential between Oxygen Molecules. Journal of the Physical Society of Japan, 2013, 82, 093701.	0.7	20
268	Origin of the band dispersion in a metal phthalocyanine crystal. Physical Review B, 2014, 90, .	1.1	15
269	Typeâ€Dependent Identification of DNA Nucleobases by Using Diamondoids. ChemPhysChem, 2014, 15, 3466-3475.	1.0	3
270	First Principles Methods: A Perspective from Quantum Monte Carlo. Entropy, 2014, 16, 287-321.	1.1	33
271	van der Waals density functionals built upon the electron-gas tradition: Facing the challenge of competing interactions. Journal of Chemical Physics, 2014, 140, 18A539.	1.2	100
272	Communication: Ab initio simulations of hydrogen-bonded ferroelectrics: Collective tunneling and the origin of geometrical isotope effects. Journal of Chemical Physics, 2014, 140, 041103.	1.2	19

#	Article	IF	Citations
273	Benchmarking exchange-correlation functionals for hydrogen at high pressures using quantum Monte Carlo. Physical Review B, 2014, 89, .	1.1	72
274	Comparison of van der Waals corrected and sparse-matter density functionals for the metal-free phthalocyanine/gold interface. Physical Review B, 2014, 89, .	1.1	38
275	Adsorption of CO2, N2, and CH4 in Cs-exchanged chabazite: A combination of van der Waals density functional theory calculations and experiment study. Journal of Chemical Physics, 2014, 140, 084705.	1.2	43
276	Noble gas encapsulation into carbon nanotubes: Predictions from analytical model and DFT studies. Journal of Chemical Physics, 2014, 141, 184304.	1.2	17
277	A van der Waals density functional theory comparison of metal decorated graphene systems for hydrogen adsorption. Journal of Applied Physics, 2014, 115, 224301.	1.1	35
278	Recommending Hartreeâ€“Fock Theory with London-Dispersion and Basis-Set-Superposition Corrections for the Optimization or Quantum Refinement of Protein Structures. Journal of Physical Chemistry B, 2014, 118, 14612-14626.	1.2	53
279	On-surface synthesis of a two-dimensional porous coordination network: Unraveling adsorbate interactions. Physical Review B, 2014, 90, .	1.1	61
280	Do Agn (up to n = 8) clusters retain their identity on graphite? Insights from first-principles calculations including dispersion interactions. Journal of Chemical Physics, 2014, 140, 164705.	1.2	13
281	Including screening in van der Waals corrected density functional theory calculations: The case of atoms and small molecules physisorbed on graphene. Journal of Chemical Physics, 2014, 140, 124107.	1.2	61
282	Diamondoids as DNA methylation and mutation probes. Europhysics Letters, 2014, 108, 17005.	0.7	6
283	Modeling the adsorption of short alkanes in the zeolite SSZ-13 using â€œvan der Waalsâ€•DFT exchange correlation functionals: Understanding the advantages and limitations of such functionals. Journal of Chemical Physics, 2014, 140, 154105.	1.2	21
284	Testing several recent van der Waals density functionals for layered structures. Journal of Chemical Physics, 2014, 141, 074708.	1.2	145
285	Phonon thermal transport in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Bi</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">Te</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>from first principles. Physical Review B, 2014, 90, .	1.1	150
286	Evaluating interaction energies of weakly bonded systems using the Buckingham-Hirshfeld method. Journal of Chemical Physics, 2014, 140, 184105.	1.2	5
287	Insight into the description of van der Waals forces for benzene adsorption on transition metal (111) surfaces. Journal of Chemical Physics, 2014, 140, 084704.	1.2	158
288	Li intercalation in graphite: A van der Waals density-functional study. Physical Review B, 2014, 90, .	1.1	63
289	Promoting the assembly of carbon onions: An atomistic approach. Physica Status Solidi (A) Applications and Materials Science, 2014, 211, 277-287.	0.8	4
290	First-principles predicted low-energy structures of NaSc(BH4)4. Journal of Chemical Physics, 2014, 140, 124708.	1.2	25

#	Article	IF	Citations
291	The role of a diamondoid as a hydrogen donor or acceptor in probing DNA nucleobases. European Physical Journal E, 2014, 37, 95.	0.7	9
292	Adsorption of Large Hydrocarbons on Coinage Metals: A van der Waals Density Functional Study. ChemPhysChem, 2014, 15, 2851-2858.	1.0	45
293	Revisiting the adsorption of copper-phthalocyanine on Au(111) including van der Waals corrections. Journal of Chemical Physics, 2014, 140, 124711.	1.2	11
294	Exchange functional that tests the robustness of the plasmon description of the van der Waals density functional. Physical Review B, 2014, 89, .	1.1	414
295	Assessments of Semilocal Density Functionals and Corrections for Carbon Dioxide Adsorption on Metalâ€“Organic Frameworks. ChemPhysChem, 2014, 15, 3157-3165.	1.0	11
297	From Doubleâ€Fourâ€Ring Germanosilicates to New Zeolites: In Silico Investigation. ChemPhysChem, 2014, 15, 2972-2976.	1.0	31
298	Predicting adsorption enthalpies on silicalite and HZSMâ€5: A benchmark study on DFT strategies addressing dispersion interactions. Journal of Computational Chemistry, 2014, 35, 809-819.	1.5	31
299	Divide-and-conquer quantum mechanical material simulations with exascale supercomputers. National Science Review, 2014, 1, 604-617.	4.6	14
300	Linear Response Methods in Quantum Chemistry. Letters in Mathematical Physics, 2014, , 97-110.	0.4	7
301	Interaction of silicene withÎ²-Si₃N₄(0001)/Si(111) substrate; energetics and electronic properties. Journal of Physics Condensed Matter, 2014, 26, 395009.	0.7	6
302	Squeezing water clusters between graphene sheets: energetics, structure, and intermolecular interactions. Physical Chemistry Chemical Physics, 2014, 16, 26004-26015.	1.3	12
303	Chiral surface networks of 3-HPLN â€" A molecular analog of rounded triangle assembly. Surface Science, 2014, 629, 65-74.	0.8	7
304	Identifying the nature of interaction between LiBH4 and two-dimensional substrates: DFT study with van der Waals correction. Journal of Alloys and Compounds, 2014, 587, 428-436.	2.8	4
305	Quantum-Informed Multiscale M&S for Energetic Materials. Advances in Quantum Chemistry, 2014, 69, 171-219.	0.4	14
306	Quest for a universal density functional: the accuracy of density functionals across a broad spectrum of databases in chemistry and physics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20120476.	1.6	599
307	Defect engineering of graphene for effective hydrogen storage. International Journal of Hydrogen Energy, 2014, 39, 4981-4995.	3.8	96
308	Towards Design Rules for Covalent Nanostructures on Metal Surfaces. Chemistry - A European Journal, 2014, 20, 928-934.	1.7	68
309	The classical molecular dynamics simulation of graphene on Ru(0001) using a fitted Tersoff interface potential. Surface and Interface Analysis, 2014, 46, 42-47.	0.8	6

#	Article	IF	Citations
310	How Do DFT-DCP, DFT-NL, and DFT-D3 Compare for the Description of London-Dispersion Effects in Conformers and General Thermochemistry?. Journal of Chemical Theory and Computation, 2014, 10, 968-980.	2.3	81
311	Methane Storage in Metal-Substituted Metalâ€“Organic Frameworks: Thermodynamics, Usable Capacity, and the Impact of Enhanced Binding Sites. Journal of Physical Chemistry C, 2014, 118, 2929-2942.	1.5	43
312	Chemically modified diamondoids as biosensors for DNA. Nanoscale, 2014, 6, 4225-4232.	2.8	20
313	Understanding the Fundamental Role of Ï€/Ï€, Ïƒ/Ïƒ, and Ïƒ/Ï€ Dispersion Interactions in Shaping Carbonâ€Based Materials. Chemistry - A European Journal, 2014, 20, 4931-4941.	1.7	109
314	Lattice matching and electronic structure of finite-layer graphene/<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>h</mml:mi></mml:math>-BN thin films. Physical Review B, 2014, 89, .	1.1	21
315	Si(111)2Ã—1 surface isomers: DFT investigations on stability and doping effects. Surface Science, 2014, 621, 123-127.	0.8	6
316	Energy Decomposition Scheme Based on the Generalized Kohnâ€“Sham Scheme. Journal of Physical Chemistry A, 2014, 118, 2531-2542.	1.1	130
317	A study of planar anchor groups for graphene-based single-molecule electronics. Journal of Chemical Physics, 2014, 140, 054708.	1.2	37
318	Resonant Raman scattering of graphite intercalation compounds KC₈, KC₂₄, and KC₃₆. Journal of Raman Spectroscopy, 2014, 45, 219-223.	1.2	15
319	DFT-D investigation of the interaction between Ir (III) based photosensitizers and small silver clusters Agn (n=2â€“20,92). Chemical Physics, 2014, 435, 40-48.	0.9	10
320	Perspective: Fifty years of density-functional theory in chemical physics. Journal of Chemical Physics, 2014, 140, 18A301.	1.2	1,083
321	Growth of epitaxial graphene: Theory and experiment. Physics Reports, 2014, 542, 195-295.	10.3	228
322	Accurate Thermochemistry for Large Molecules with Modern Density Functionals. Topics in Current Chemistry, 2014, , 1-23.	4.0	17
323	Assessing electronic structure approaches for gas-ligand interactions in metal-organic frameworks: The CO2-benzene complex. Journal of Chemical Physics, 2014, 140, 104707.	1.2	20
324	Evaluation of model exchange-correlation kernels in the adiabatic connection fluctuation-dissipation theorem for inhomogeneous systems. Journal of Chemical Physics, 2014, 140, 18A520.	1.2	26
325	Exploring the limit of accuracy for density functionals based on the generalized gradient approximation: Local, global hybrid, and range-separated hybrid functionals with and without dispersion corrections. Journal of Chemical Physics, 2014, 140, 18A527.	1.2	34
326	Two-Dimensional Zeolites: Current Status and Perspectives. Chemical Reviews, 2014, 114, 4807-4837.	23.0	625
327	First-principles investigation of the bulk and low-index surfaces of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Mo</mml:mi><mml:msub><mml:mi>Se</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review B, 2014, 89, .	1.1	19

#	Article	IF	Citations
328	Study of van der Waals bonding and interactions in metal organic framework materials. Journal of Physics Condensed Matter, 2014, 26, 133002.	0.7	34
329	Theoretical investigation of layered zeolite frameworks: Surface properties of 2D zeolites. Catalysis Today, 2014, 227, 2-8.	2.2	25
330	Optimizing the Band Edges of Tungsten Trioxide for Water Oxidation: A First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 6019-6028.	1.5	63
331	Design of a Metalâ€“Organic Framework with Enhanced Back Bonding for Separation of N₂ and CH₄. Journal of the American Chemical Society, 2014, 136, 698-704.	6.6	157
332	Density Functional Theory of Open-Shell Systems. The 3d-Series Transition-Metal Atoms and Their Cations. Journal of Chemical Theory and Computation, 2014, 10, 102-121.	2.3	65
333	Error Estimates for Solid-State Density-Functional Theory Predictions: An Overview by Means of the Ground-State Elemental Crystals. Critical Reviews in Solid State and Materials Sciences, 2014, 39, 1-24.	6.8	404
334	Computational studies of charge transfer in organic solar photovoltaic cells: A review. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2014, 18, 18-31.	5.6	33
335	Recent developments in first-principles force fields for molecules in nanoporous materials. Journal of Materials Chemistry A, 2014, 2, 274-291.	5.2	126
336	Molecular phenomena in colloidal nanostructure synthesis. Molecular Simulation, 2014, 40, 134-140.	0.9	14
337	Measuring the BrÃ¸nsted acid strength of zeolites â€“ does it correlate with the Oâ€“H frequency shift probed by a weak base?. Physical Chemistry Chemical Physics, 2014, 16, 10129-10141.	1.3	62
338	DNA-based nanobiostructured devices: The role of quasiperiodicity and correlation effects. Physics Reports, 2014, 535, 139-209.	10.3	88
339	A van der Waals density functional study of the adsorption of ethanol on the Î±-alumina (0001) surface. Surface Science, 2014, 621, 16-22.	0.8	9
340	Correcting density functionals for dispersion interactions using pseudopotentials. Chemical Physics Letters, 2014, 591, 133-136.	1.2	17
341	Assessing the Performances of Dispersion-Corrected Density Functional Methods for Predicting the Crystallographic Properties of High Nitrogen Energetic Salts. Journal of Chemical Theory and Computation, 2014, 10, 4982-4994.	2.3	22
342	On the role of long range interactions for the adsorption of sexithiophene on Ag(110) surface. Journal of Chemical Physics, 2014, 140, 144703.	1.2	16
343	Binding and Diffusion of Lithium in Graphite: Quantum Monte Carlo Benchmarks and Validation of van der Waals Density Functional Methods. Journal of Chemical Theory and Computation, 2014, 10, 5318-5323.	2.3	117
344	First-Principles Analysis of Defect-Mediated Li Adsorption on Graphene. ACS Applied Materials & Interfaces, 2014, 6, 21141-21150.	4.0	120
345	Water on BN doped benzene: A hard test for exchange-correlation functionals and the impact of exact exchange on weak binding. Journal of Chemical Physics, 2014, 141, 18C530.	1.2	25

#	Article	IF	Citations
346	Arginine-phosphate salt bridges between histones and DNA: Intermolecular actuators that control nucleosome architecture. Journal of Chemical Physics, 2014, 141, 165102.	1.2	19
347	Costless Derivation of Dispersion Coefficients for Metal Surfaces. Journal of Chemical Theory and Computation, 2014, 10, 5002-5009.	2.3	49
348	Kinetic, Spectroscopic, and Theoretical Assessment of Associative and Dissociative Methanol Dehydration Routes in Zeolites. Angewandte Chemie - International Edition, 2014, 53, 12177-12181.	7.2	122
349	Achievements of DFT for the Investigation of Graphene-Related Nanostructures. Accounts of Chemical Research, 2014, 47, 3292-3300.	7.6	15
350	Modeling Catalytic Steps on Extra-Framework Metal Centers in Zeolites. A Case Study on Ethylene Dimerization. Journal of Physical Chemistry C, 2014, 118, 25077-25088.	1.5	16
351	Single-Layer MoS₂ with Sulfur Vacancies: Structure and Catalytic Application. Journal of Physical Chemistry C, 2014, 118, 5346-5351.	1.5	260
352	Interpretation of van der Waals density functionals. Physical Review B, 2014, 90, .	1.1	63
353	Benchmarking Calculated Lattice Parameters and Energies of Molecular Crystals Using van der Waals Density Functionals. Journal of Chemical Theory and Computation, 2014, 10, 3423-3437.	2.3	56
354	Efficient simulations of the aqueous bio-interface of graphitic nanostructures with a polarisable model. Nanoscale, 2014, 6, 5438-5448.	2.8	62
355	Theoretical investigation of layered zeolites with MWW topology: MCM-22P vs. MCM-56. Dalton Transactions, 2014, 43, 10443-10450.	1.6	33
356	Periodic MP2, RPA, and Boundary Condition Assessment of Hydrogen Ordering in Ice XV. Journal of Physical Chemistry Letters, 2014, 5, 4122-4128.	2.1	48
357	Oxalyl dihydrazide polymorphism: a periodic dispersion-corrected DFT and MP2 investigation. CrystEngComm, 2014, 16, 102-109.	1.3	23
358	Density Functional Theory Based Study of Molecular Interactions, Recognition, Engineering, and Quantum Transport in Ï€ Molecular Systems. Accounts of Chemical Research, 2014, 47, 3321-3330.	7.6	54
359	Verification of the dual cycle mechanism for methanol-to-olefin conversion in HSAPO-34: a methylbenzene-based cycle from DFT calculations. Catalysis Science and Technology, 2014, 4, 2631-2638.	2.1	54
360	Van der Waals density functional study of the energetics of alkali metal intercalation in graphite. RSC Advances, 2014, 4, 3973-3983.	1.7	145
361	Calculating NMR parameters in aluminophosphates: evaluation of dispersion correction schemes. Physical Chemistry Chemical Physics, 2014, 16, 2660.	1.3	32
362	Ligand Effects on the Regioselectivity of Rhodium-Catalyzed Hydroformylation: Density Functional Calculations Illuminate the Role of Long-Range Noncovalent Interactions. Organometallics, 2014, 33, 4183-4191.	1.1	47
363	Efficient Determination of Accurate Force Fields for Porous Materials Using ab Initio Total Energy Calculations. Journal of Physical Chemistry C, 2014, 118, 2693-2701.	1.5	23

#	Article	IF	Citations
364	Assessing the reliability of calculated catalytic ammonia synthesis rates. Science, 2014, 345, 197-200.	6.0	319
365	Structures, Mechanical Properties, Equations of State, and Electronic Properties of Î²-HMX under Hydrostatic Pressures: A DFT-D2 study. Physical Chemistry Chemical Physics, 2014, 16, 19972-83.	1.3	42
366	van der Waals effects at molecule-metal interfaces. Physical Review B, 2014, 90, .	1.1	22
367	Ï‰B97X-V: A 10-parameter, range-separated hybrid, generalized gradient approximation density functional with nonlocal correlation, designed by a survival-of-the-fittest strategy. Physical Chemistry Chemical Physics, 2014, 16, 9904.	1.3	616
368	Extending the applicability of the Tkatchenko-Scheffler dispersion correction via iterative Hirshfeld partitioning. Journal of Chemical Physics, 2014, 141, 034114.	1.2	174
369	Density Functional Theory with van der Waals Corrections Study of the Adsorption of Alkyl, Alkylthiol, Alkoxyl, and Amino-Alkyl Chains on the H:Si(111) Surface. Langmuir, 2014, 30, 13255-13265.	1.6	14
370	Comprehensive study of carbon dioxide adsorption in the metalâ€“organic frameworks M₂(dobdc) (M = Mg, Mn, Fe, Co, Ni, Cu, Zn). Chemical Science, 2014, 5, 4569-4581.	3.7	342
371	Particle size and hydration medium effects on hydration properties and sugar release of wheat straw fibers. Biomass and Bioenergy, 2014, 68, 67-74.	2.9	14
372	Parametrization of a classical force field for iron oxyhydroxide/water interfaces based on Density Functional Theory calculations. Computational Materials Science, 2014, 92, 343-352.	1.4	15
373	Self-consistent relativistic band structure of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">CH</mml:mi><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">NH</mml:mi><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">PbI</mml:mi><mml:msub><mml:mrow	1.1	245
374	Catalysis by Dynamically Formed Defects in a Metalâ€“Organic Framework Structure: Knoevenagel Reaction Catalyzed by Copper Benzeneâ€1,3,5â€tricarboxylate. ChemCatChem, 2014, 6, 2821-2824.	1.8	54
375	Understanding the Interface of Liquids with an Organic Crystal Surface from Atomistic Simulations and AFM Experiments. Journal of Physical Chemistry C, 2014, 118, 2058-2066.	1.5	23
376	Microstructure-Dependent Gas Adsorption: Accurate Predictions of Methane Uptake in Nanoporous Carbons. Journal of Chemical Theory and Computation, 2014, 10, 1-4.	2.3	22
377	Adsorption of tetrathiafulvalene (TTF) on Cu(1 0 0): can Ï€-stacked 1-D aggregates be formed at low temperature?. Chemical Physics Letters, 2014, 612, 45-50.	1.2	0
378	Strain-Induced Gap Modification in Black Phosphorus. Physical Review Letters, 2014, 112, 176801.	2.9	1,303
379	Effects of van der Waals interactions and quasiparticle corrections on the electronic and transport properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Bi</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">Te</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 90, .	1.1	63
381	van der <scp>W</scp>aals corrected density functional calculations of the adsorption of benzene on the Cu (111) surface. Journal of Computational Chemistry, 2014, 35, 2263-2271.	1.5	11
382	Spin-Component-Scaled Double-Hybrid Density Functionals with Nonlocal van der Waals Correlations for Noncovalent Interactions. Journal of Chemical Theory and Computation, 2014, 10, 4400-4407.	2.3	39

#	Article	IF	Citations
383	Range-Separated meta-GGA Functional Designed for Noncovalent Interactions. Journal of Chemical Theory and Computation, 2014, 10, 4297-4306.	2.3	17
384	Charge transport and rectification in molecular junctions formed with carbon-based electrodes. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 10928-10932.	3.3	95
385	exciting: a full-potential all-electron package implementing density-functional theory and many-body perturbation theory. Journal of Physics Condensed Matter, 2014, 26, 363202.	0.7	241
386	Hydration structure of Na⁺and K⁺fromab initiomolecular dynamics based on modern density functional theory. Molecular Physics, 2014, 112, 1448-1456.	0.8	37
387	Phosphonic Acid Adsorbates Tune the Surface Potential of TiO₂ in Gas and Liquid Environments. Journal of Physical Chemistry Letters, 2014, 5, 2450-2454.	2.1	15
388	Density Functional Investigation of the Adsorption of Isooctane, Ethanol, and Acetic Acid on a Water-Covered Fe(100) Surface. Journal of Physical Chemistry C, 2014, 118, 21428-21437.	1.5	17
389	Intrinsic Ligand Effect Governing the Catalytic Activity of Pd Oxide Thin Films. ACS Catalysis, 2014, 4, 3330-3334.	5.5	79
390	DFT investigation of the vibrational properties of GC Watson-Crick and Hoogsteen base pairs in the presence of Mg2+, Ca2+, and Cu2+ ions. Journal of Molecular Modeling, 2014, 20, 2220.	0.8	4
391	Physical Adsorption and Charge Transfer of Molecular Br₂ on Graphene. ACS Nano, 2014, 8, 2943-2950.	7.3	58
392	Development of a â€œFirst Principlesâ€•Water Potential with Flexible Monomers. II: Trimer Potential Energy Surface, Third Virial Coefficient, and Small Clusters. Journal of Chemical Theory and Computation, 2014, 10, 1599-1607.	2.3	313
393	Mechanisms of the Adsorption and Self-Assembly of Molecules with Polarized Functional Groups on Insulating Surfaces. Journal of Physical Chemistry C, 2014, 118, 14569-14578.	1.5	28
394	Effect of van der Waals interaction on the structural and cohesive properties of black phosphorus. Journal of the Korean Physical Society, 2014, 64, 547-553.	0.3	21
395	Self-assembly of carbon nanoclusters on dielectric boron nitride. Applied Surface Science, 2014, 292, 237-246.	3.1	3
396	Adsorption of CO2 in FAU zeolites: Effect of zeolite composition. Catalysis Today, 2014, 227, 50-56.	2.2	80
397	Force-Field Development from Electronic Structure Calculations with Periodic Boundary Conditions: Applications to Gaseous Adsorption and Transport in Metalâ€“Organic Frameworks. Journal of Chemical Theory and Computation, 2014, 10, 1477-1488.	2.3	121
398	Long-range correlation energy calculated from coupled atomic response functions. Journal of Chemical Physics, 2014, 140, 18A508.	1.2	480
399	Density functional theory: Foundations reviewed. Physics Reports, 2014, 544, 123-239.	10.3	91
400	Reversible CO Binding Enables Tunable CO/H₂ and CO/N₂ Separations in Metalâ€“Organic Frameworks with Exposed Divalent Metal Cations. Journal of the American Chemical Society, 2014, 136, 10752-10761.	6.6	210

#	Article	IF	Citations
401	Interaction of H₂ with a Double-Walled Armchair Nanotube by First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 15816-15824.	1.5	5
402	van der Waals density functional made accurate. Physical Review B, 2014, 89, .	1.1	524
403	First-principles study of van der Waals interactions in MoS₂and MoO₃. Journal of Physics Condensed Matter, 2014, 26, 305502.	0.7	45
404	Thermally Controlled Adenine Dimer Chain Rotation on Cu(110): The Critical Role of van der Waals Interactions. Journal of Physical Chemistry C, 2014, 118, 6278-6282.	1.5	7
405	Implications of Transition State Confinement within Small Voids for Acid Catalysis. Journal of Physical Chemistry C, 2014, 118, 17787-17800.	1.5	115
406	Computational Investigation of the Lewis Acidity in Three-Dimensional and Corresponding Two-Dimensional Zeolites: UTL vs IPC-1P. Journal of Physical Chemistry A, 2014, 118, 7526-7534.	1.1	16
407	Multiphase equation of state for carbon addressing high pressures and temperatures. Physical Review B, 2014, 89, .	1.1	127
408	Benchmarking van der Waals functionals with noncontact RPA calculations on graphene-Ag(111). Physical Review B, 2014, 90, .	1.1	33
409	Plane-wave density functional theory investigation of adsorption of 2,4,6-trinitrotoluene on al-hydroxylated (0001) surface of (4 Ã— 4) Î±-alumina. Journal of Computational Chemistry, 2014, 35, 1977-1985.	1.5	7
410	Gas Separation in Nanoporous Graphene from First Principle Calculations. Journal of Physical Chemistry C, 2014, 118, 19172-19179.	1.5	63
411	Effects of van der Waals Interactions in the Adsorption of Isooctane and Ethanol on Fe(100) Surfaces. Journal of Physical Chemistry C, 2014, 118, 17608-17615.	1.5	61
412	Configurational Entropy in Ice Nanosystems: Tools for Structure Generation and Screening. Journal of Chemical Theory and Computation, 2014, 10, 1256-1264.	2.3	2
413	Effect of dispersion on surface interactions of cobalt(<scp>ii</scp>) octaethylporphyrin monolayer on Au(111) and HOPG(0001) substrates: a comparative first principles study. Physical Chemistry Chemical Physics, 2014, 16, 14096-14107.	1.3	58
414	Many-body van der Waals interactions in molecules and condensed matter. Journal of Physics Condensed Matter, 2014, 26, 213202.	0.7	190
415	Effect of strain on atomic-scale friction in layered MoS2. Tribology International, 2014, 77, 211-217.	3.0	33
416	DFT study of the trioxotriangulene derivatives in bulk state. Chemical Physics Letters, 2014, 598, 48-52.	1.2	4
417	Hydrostatic pressure effects on structural and electronic properties of TATB from first principles calculations. Chemical Physics, 2014, 436-437, 1-7.	0.9	30
418	Structural Correspondence of Solution, Liquid Crystal, and Crystalline Phases of the Chromonic Mesogen Sunset Yellow. Crystal Growth and Design, 2014, 14, 4166-4176.	1.4	21

#	Article	IF	Citations
419	Quantum Monte Carlo Benchmark of Exchange-Correlation Functionals for Bulk Water. Journal of Chemical Theory and Computation, 2014, 10, 2355-2362.	2.3	39
420	Modeling Adsorption and Reactions of Organic Molecules at Metal Surfaces. Accounts of Chemical Research, 2014, 47, 3369-3377.	7.6	218
421	Interplay of hydrogen bonding and moleculeâ€“substrate interaction in self-assembled adlayer structures of a hydroxyphenyl-substituted porphyrin. Surface Science, 2014, 628, 132-140.	0.8	20
422	Predicting the Relative Solubilities of Racemic and Enantiopure Crystals by Densityâ€Functional Theory. Angewandte Chemie - International Edition, 2014, 53, 7879-7882.	7.2	56
423	Adsorption of small aromatic molecules on gold: a DFT localized basis set study including van der Waals effects. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	33
424	First-principles insights into the electronic and magnetic structure of hybrid organic-metal interfaces. Journal of Physics Condensed Matter, 2014, 26, 263001.	0.7	10
425	Gas Membrane Selectivity Enabled by Zeolitic Imidazolate Framework Electrostatics. Chemistry of Materials, 2014, 26, 3976-3985.	3.2	25
426	Understanding the Adsorption of CuPc and ZnPc on Noble Metal Surfaces by Combining Quantum-Mechanical Modelling and Photoelectron Spectroscopy. Molecules, 2014, 19, 2969-2992.	1.7	69
427	The effect of the exchange-correlation functional on H2 dissociation on Ru(0001). Journal of Chemical Physics, 2014, 140, 084702.	1.2	57
428	Nuclear quantum effects in a 1-D model of hydrogen bonded ferroelectrics. Journal of Physics: Conference Series, 2014, 571, 012012.	0.3	7
429	Effect of Incorporating Aromatic and Chiral Groups on the Dielectric Properties of Poly(dimethyltin) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	2.0	29
431	Thermal diffusion of correlated Li-ions in graphite: A hybrid quantumâ€“classical simulation study. Computational Materials Science, 2015, 108, 250-257.	1.4	4
432	Prediction of the Xeâ€“He binary phase diagram at high pressures. Chemical Physics Letters, 2015, 640, 115-118.	1.2	11
433	Structures and vibrational frequencies of CO adsorbed on transition metals from calculations using the vdW-DF2 functional. Computational and Theoretical Chemistry, 2015, 1069, 147-154.	1.1	16
434	Electronic properties of GaSe, InSe, GaS and GaTe layered semiconductors: charge neutrality level and interface barrier heights. Semiconductor Science and Technology, 2015, 30, 115019.	1.0	34
435	Finding the right substrate support for magnetic superatom assembly from density functional calculations. Physical Review B, 2015, 91, .	1.1	4
436	Surface energetics of alkaline-earth metal oxides: Trends in stability and adsorption of small molecules. Physical Review B, 2015, 91, .	1.1	41
437	Assessing the accuracy of the van der Waals density functionals for rare-gas and small molecular systems. Physical Review B, 2015, 91, .	1.1	34

#	Article	IF	Citations
438	Adsorption of metal nanoparticles on carbon substrates and epitaxial graphene: Assessing models for dispersion forces. Physical Review B, 2015, 91, .	1.1	9
439	van der Waals bilayer energetics: Generalized stacking-fault energy of graphene, boron nitride, and graphene/boron nitride bilayers. Physical Review B, 2015, 92, .	1.1	105
440	Spin Signature of Nonlocal Correlation Binding in Metal-Organic Frameworks. Physical Review Letters, 2015, 115, 136402.	2.9	272
441	Nature of the Volume Isotope Effect in Ice. Physical Review Letters, 2015, 115, 173005.	2.9	22
442	van der Waals corrected DFT simulation of adsorption processes on transition-metal surfaces: Xe and graphene on Ni(111). Physical Review B, 2015, 91, .	1.1	39
443	Structural diversity in lithium carbides. Physical Review B, 2015, 92, .	1.1	26
444	Tuning the van der Waals Interaction of Graphene with Molecules via Doping. Physical Review Letters, 2015, 115, 236101.	2.9	48
445	Layer-selective half-metallicity in bilayer graphene nanoribbons. Scientific Reports, 2015, 5, 9825.	1.6	10
446	Structural, electronic and vibrational properties of few-layer 2H- and 1T-TaSe2. Scientific Reports, 2015, 5, 16646.	1.6	44
447	Influence of the exchange-correlation functional on the quasi-harmonic lattice dynamics of II-VI semiconductors. Journal of Chemical Physics, 2015, 143, 064710.	1.2	80
448	Optical signatures of bulk and solutions of KC8 and KC24. Journal of Applied Physics, 2015, 118, 044304.	1.1	8
449	Computational phase diagrams of noble gas hydrates under pressure. Journal of Chemical Physics, 2015, 143, 154507.	1.2	30
450	An energy decomposition analysis for second-order MÃ¸llerâ€“Plesset perturbation theory based on absolutely localized molecular orbitals. Journal of Chemical Physics, 2015, 143, 084124.	1.2	48
451	Electron transport in molecular junctions with graphene as protecting layer. Journal of Chemical Physics, 2015, 143, 214302.	1.2	6
453	N2 dissociation on W(110): An ab initio molecular dynamics study on the effect of phonons. Journal of Chemical Physics, 2015, 142, 104702.	1.2	22
454	Transferability and accuracy by combining dispersionless density functional and incremental post-Hartree-Fock theories: Noble gases adsorption on coronene/graphene/graphite surfaces. Journal of Chemical Physics, 2015, 143, 194701.	1.2	34
455	Understanding Smallâ€Molecule Interactions in Metalâ€“Organic Frameworks: Coupling Experiment with Theory. Advanced Materials, 2015, 27, 5785-5796.	11.1	33
456	Ammine Calcium and Strontium Borohydrides: Syntheses, Structures, and Properties. ChemSusChem, 2015, 8, 3472-3482.	3.6	24

#	Article	IF	Citations
457	Dissolution on Titan and on Earth: Toward the age of Titan's karstic landscapes. Journal of Geophysical Research E: Planets, 2015, 120, 1044-1074.	1.5	63
458	Structural Properties of Liquid Water and Ice Ih from Ab-Initio Molecular Dynamics with a Non-Local Correlation Functional. Energies, 2015, 8, 9383-9391.	1.6	20
459	Similarities and differences between aromatic-based and olefin-based cycles in H-SAPO-34 and H-SSZ-13 for methanol-to-olefins conversion: insights from energetic span model. Catalysis Science and Technology, 2015, 5, 4354-4364.	2.1	87
460	Molecular to Atomic Phase Transition in Hydrogen under High Pressure. Physical Review Letters, 2015, 114, 105305.	2.9	123
461	Predicting Methane Storage in Open-Metal-Site Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2015, 119, 13451-13458.	1.5	62
462	Application of a VanÂDerÂWaals Density Functional to Small Molecular Complexes and Solids. , 2015, , .		1
463	Energy landscape and band-structure tuning in realistic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2015, 91, .	1.1	47
464	Methane adsorption on intrinsic, vacancy and N-doped graphene: A first-principles study. Physica Status Solidi (B): Basic Research, 2015, 252, 1757-1766.	0.7	13
465	Density and Compressibility of Liquid Water and Ice from First-Principles Simulations with Hybrid Functionals. Journal of Physical Chemistry Letters, 2015, 6, 2902-2908.	2.1	77
466	Subsystem-DFT potential-energy curves for weakly interacting systems. Physical Chemistry Chemical Physics, 2015, 17, 14323-14341.	1.3	33
467	van der Waals dispersion interactions in molecular materials: beyond pairwise additivity. Chemical Science, 2015, 6, 3289-3301.	3.7	172
468	Two-dimensional Kagome phosphorus and its edge magnetism: a density functional theory study. Journal of Physics Condensed Matter, 2015, 27, 255006.	0.7	16
469	First Principles Study on Solid Oxygen Using Van Der Waals Density Functional. Physics Procedia, 2015, 75, 771-778.	1.2	2
470	Silicene on MoS ₂ : role of the van der Waals interaction. 2D Materials, 2015, 2, 045004.	2.0	22
471	Quasi-Free-Standing Features of Stanene/Stanane on InSe and GaTe Nanosheets: A Computational Study. Journal of Physical Chemistry C, 2015, 119, 27848-27854.	1.5	24
472	Hindered rotational physisorption states of H2 on Ag(111) surfaces. Physical Chemistry Chemical Physics, 2015, 17, 19625-19630.	1.3	3
473	Accelerated materials property predictions and design using motif-based fingerprints. Physical Review B, 2015, 92, .	1.1	136
474	Kinetically Trapped Two-Component Self-Assembled Adlayer. Journal of Physical Chemistry C, 2015, 119, 25364-25376.	1.5	27

#	Article	IF	Citations
475	The Nonlocal Correlation Density Functional VV10. Annual Reports in Computational Chemistry, 2015, 11, 37-102.	0.9	17
476	Improving the Description of Nonmagnetic and Magnetic Molecular Crystals via the van der Waals Density Functional. Journal of the Physical Society of Japan, 2015, 84, 024715.	0.7	14
477	Structure, Activity, and Deactivation Mechanisms in Double Metal Cyanide Catalysts for the Production of Polyols. ChemCatChem, 2015, 7, 928-935.	1.8	34
478	Water adsorption in metalâ€“organic frameworks with openâ€metal sites. AICHE Journal, 2015, 61, 677-687.	1.8	37
479	First-Principles Study of Redox End Members in Lithiumâ€“Sulfur Batteries. Journal of Physical Chemistry C, 2015, 119, 4675-4683.	1.5	65
480	Design of electrocatalysts for oxygen- and hydrogen-involving energy conversion reactions. Chemical Society Reviews, 2015, 44, 2060-2086.	18.7	4,323
481	Tetrahydrothiophene and Tetrahydrofuran, Computational and X-ray Studies in the Crystalline Phase. Crystal Growth and Design, 2015, 15, 1073-1081.	1.4	15
482	Density Functional Theory and Hydrogen Bonds: Are We There Yet?. ChemPhysChem, 2015, 16, 978-985.	1.0	129
483	Dispersion Correction Derived from First Principles for Density Functional Theory and Hartreeâ€“Fock Theory. Journal of Physical Chemistry A, 2015, 119, 2161-2168.	1.1	17
484	Choosing a density functional for modeling adsorptive hydrogen storage: reference quantum mechanical calculations and a comparison of dispersion-corrected density functionals. Physical Chemistry Chemical Physics, 2015, 17, 6423-6432.	1.3	33
485	Performance of Dispersion-Corrected DFT for the Weak Interaction between Aromatic Molecules and Extended Carbon-Based Systems. Journal of Physical Chemistry C, 2015, 119, 1898-1904.	1.5	37
486	Chemical insight from density functional modeling of molecular adsorption: Tracking the bonding and diffusion of anthracene derivatives on Cu(111) with molecular orbitals. Journal of Chemical Physics, 2015, 142, 101907.	1.2	7
487	Insight into the Effect of Long Range Interactions for the Adsorption of Benzene on Transition Metal (110) Surfaces. Journal of Physical Chemistry C, 2015, 119, 1886-1897.	1.5	37
488	Time-lapsed graphene moirÃ© superlattices on Cu(1â€‰1â€‰1). Modelling and Simulation in Materials Science and Engineering, 2015, 23, 025001.	0.8	8
489	Vibrational mode frequencies of H2S and H2O adsorbed on Ge(001)-(2Ã—1) surfaces. Applied Surface Science, 2015, 329, 363-370.	3.1	6
490	Theoretical modeling of friction and wear processes at atomic level. , 2015, , 385-405.		4
491	Scrutinizing individual CoTPP molecule adsorbed on coinage metal surfaces from the interplay of STM experiment and theory. Surface Science, 2015, 635, 108-114.	0.8	12
492	Small-Molecule Adsorption in Open-Site Metalâ€“Organic Frameworks: A Systematic Density Functional Theory Study for Rational Design. Chemistry of Materials, 2015, 27, 668-678.	3.2	248

#	Article	IF	Citations
493	AIREBO-M: A reactive model for hydrocarbons at extreme pressures. Journal of Chemical Physics, 2015, 142, 024903.	1.2	159
494	Isobaric first-principles molecular dynamics of liquid water with nonlocal van der Waals interactions. Journal of Chemical Physics, 2015, 142, 034501.	1.2	68
495	Boron-Doped, Nitrogen-Doped, and Codoped Graphene on Cu(111): A DFT + vdW Study. Journal of Physical Chemistry C, 2015, 119, 6056-6064.	1.5	63
496	Bandâ€Like Electron Transport with Recordâ€High Mobility in the TCNQ Family. Advanced Materials, 2015, 27, 2453-2458.	11.1	122
497	Exploring atomic defects in molybdenum disulphide monolayers. Nature Communications, 2015, 6, 6293.	5.8	1,124
498	Direct and Indirect Effects of Dispersion Interactions on the Electric Properties of Weakly Bound Complexes. Journal of Physical Chemistry A, 2015, 119, 3112-3124.	1.1	12
499	A QM:MM model for the interaction of DNA nucleotides with carbon nanotubes. Physical Chemistry Chemical Physics, 2015, 17, 7564-7575.	1.3	19
500	Influence of the van der Waals interaction in the dissociation dynamics of N2 on W(110) from first principles. Journal of Chemical Physics, 2015, 142, 074704.	1.2	23
501	Nearly-free electronlike surface resonance of a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi><mml:mo>â^'</mml:mo><mml:msub><mml:mi mathvariant="normal">Si</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:mo>(</mml:mo><mml:mn>0001</mml:mn><mml:mo>) Physical Review B, 2015, 91, .	1.1	11
502	Cooperative insertion of CO2 in diamine-appended metal-organic frameworks. Nature, 2015, 519, 303-308.	13.7	1,026
503	Argon Interaction with Gold Surfaces: Ab Initio-Assisted Determination of Pair Arâ€“Au Potentials for Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2015, 119, 6897-6908.	1.1	18
504	DFT-Derived Force Fields for Modeling Hydrocarbon Adsorption in MIL-47(V). Langmuir, 2015, 31, 8453-8468.	1.6	37
505	The role of density functional theory methods in the prediction of nanostructured gas-adsorbent materials. Coordination Chemistry Reviews, 2015, 300, 142-163.	9.5	36
506	Adsorption of alkali adatoms on graphene supported by the Au/Ni(111) surface. Physical Review B, 2015, 92, .	1.1	30
507	First-Principles Calculation of Terahertz Absorption with Dispersion Correction of 2,2â€²-Bithiophene as Model Compound. Journal of Physical Chemistry C, 2015, 119, 12598-12607.	1.5	15
508	First-principles evaluation of multi-valent cation insertion into orthorhombic V₂O₅. Chemical Communications, 2015, 51, 13619-13622.	2.2	148
509	Range separated hybrids of pair coupled cluster doubles and density functionals. Physical Chemistry Chemical Physics, 2015, 17, 22412-22422.	1.3	40
510	Accurate Dielsâ€“Alder Reaction Energies from Efficient Density Functional Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2879-2888.	2.3	19

#	Article	IF	Citations
511	Long-range interaction of anisotropic systems. Europhysics Letters, 2015, 109, 43002.	0.7	0
512	Vibrational properties and bonding nature of Sb₂Se₃and their implications for chalcogenide materials. Chemical Science, 2015, 6, 5255-5262.	3.7	89
513	Electronic Properties of Halogen-Adsorbed Graphene. Journal of Physical Chemistry C, 2015, 119, 17271-17277.	1.5	42
514	Nitrogen Doping Enables Covalent-Like Ï€â€“Ï€ Bonding between Graphenes. Nano Letters, 2015, 15, 5482-5491.	4.5	31
515	Structural and electronic properties of MX3 (M = Ti, Zr and Hf; X = S, Se, Te) from first principles calculations. European Physical Journal B, 2015, 88, 1.	0.6	32
516	Aging mechanisms in amorphous phase-change materials. Nature Communications, 2015, 6, 7467.	5.8	212
517	Role of the dispersion force in modeling the interfacial properties of molecule-metal interfaces: adsorption of thiophene on copper surfaces. Scientific Reports, 2014, 4, 5036.	1.6	62
518	Van der Waals density functional theory study for bulk solids with BCC, FCC, and diamond structures. Current Applied Physics, 2015, 15, 885-891.	1.1	43
519	Hydrogen Activation on the Promoted and Unpromoted ReS2 (001) Surfaces under the Sulfidation Conditions: A First-Principles Study. Journal of Physical Chemistry C, 2015, 119, 17092-17101.	1.5	12
520	Reducing Systematic Errors in Oxide Species with Density Functional Theory Calculations. Journal of Physical Chemistry C, 2015, 119, 17596-17601.	1.5	29
521	Ab initio study of structural and mechanical property of solid molecular hydrogens. European Physical Journal B, 2015, 88, 1.	0.6	5
522	Trends in Syntheses, Structures, and Properties for Three Series of Ammine Rare-Earth Metal Borohydrides, M(BH₄)₃Â·nNH₃ (M = Y, Gd, and Dy). Inorganic Chemistry, 2015, 54, 7402-7414.	1.9	41
523	Electronic structures of multilayer two-dimensional silicon carbide with oriented misalignment. Journal of Materials Chemistry C, 2015, 3, 9057-9062.	2.7	27
524	Combining density functional and incremental post-Hartree-Fock approaches for van der Waals dominated adsorbate-surface interactions: Ag2/graphene. Journal of Chemical Physics, 2015, 143, 102804.	1.2	34
525	Covalent and noncovalent functionalization of pristine and defective graphene by cyclohexane and dehydrogenated derivatives. Applied Surface Science, 2015, 351, 344-352.	3.1	14
526	Single- and double-wall carbon nanotubes fully covered with tetraphenylporphyrins: Stability and optoelectronic properties from ab initio calculations. Chemical Physics Letters, 2015, 634, 47-52.	1.2	7
527	The Ab Initio Treatment of High-Pressure and High-Temperature Mineral Properties and Behavior. , 2015, , 369-392.		2
528	Direct observation of an abrupt insulator-to-metal transition in dense liquid deuterium. Science, 2015, 348, 1455-1460.	6.0	241

#	Article	IF	Citations
529	Nano-Saturn: Energetics of the Inclusion Process of C₆₀ into Cyclohexabiphenylene. Journal of Physical Chemistry C, 2015, 119, 8931-8936.	1.5	14
530	Structural, electronic and elastic properties of several metal organic frameworks as a new kind of energetic materials. Chemical Physics Letters, 2015, 628, 76-80.	1.2	13
531	Quantum-Chemical Characterization of the Properties and Reactivities of Metalâ€“Organic Frameworks. Chemical Reviews, 2015, 115, 6051-6111.	23.0	241
532	True perylene epitaxy on Ag(110) driven by site recognition effect. Journal of Chemical Physics, 2015, 142, 101929.	1.2	11
533	Understanding the Adsorption Mechanism of Xe and Kr in a Metalâ€“Organic Framework from X-ray Structural Analysis and First-Principles Calculations. Journal of Physical Chemistry Letters, 2015, 6, 1790-1794.	2.1	38
534	Mixed Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulations of Biological Systems in Ground and Electronically Excited States. Chemical Reviews, 2015, 115, 6217-6263.	23.0	352
535	Adsorption and Dissociation of H₂O on Monolayered MoS₂ Edges: Energetics and Mechanism from ab Initio Simulations. Journal of Physical Chemistry C, 2015, 119, 6518-6529.	1.5	107
536	A systematic study of metal-supported boron nitride materials for the oxygen reduction reaction. Physical Chemistry Chemical Physics, 2015, 17, 12722-12727.	1.3	65
537	van der Waals forces in density functional theory: a review of the vdW-DF method. Reports on Progress in Physics, 2015, 78, 066501.	8.1	615
538	Advances in theory and their application within the field of zeolite chemistry. Chemical Society Reviews, 2015, 44, 7044-7111.	18.7	405
539	Understanding the Anchoring Effect of Two-Dimensional Layered Materials for Lithiumâ€“Sulfur Batteries. Nano Letters, 2015, 15, 3780-3786.	4.5	779
540	Mapping the genome of meta-generalized gradient approximation density functionals: The search for B97M-V. Journal of Chemical Physics, 2015, 142, 074111.	1.2	305
541	Adsorptive desulfurization with CPO-27/MOF-74: an experimental and computational investigation. Physical Chemistry Chemical Physics, 2015, 17, 10759-10766.	1.3	47
542	Computational chemistry for graphene-based energy applications: progress and challenges. Nanoscale, 2015, 7, 6883-6908.	2.8	72
543	The energetic of (CH2F2)2 investigated by TDL IR spectroscopy and DFT computations: From collision induced relaxation of ro-vibrational transitions to non-covalent interactions. Journal of Chemical Physics, 2015, 142, 134310.	1.2	14
544	Adsorption of 2-vinyl thiophene on Si(100)2 Ã— 1: A van Der Waals corrected DFT study. Journal of Theoretical and Computational Chemistry, 2015, 14, 1550011.	1.8	4
545	The Intercalation Phase Diagram of Mg in V₂O₅ from First-Principles. Chemistry of Materials, 2015, 27, 3733-3742.	3.2	130
546	Large Frequency Change with Thickness in Interlayer Breathing Modeâ€”Significant Interlayer Interactions in Few Layer Black Phosphorus. Nano Letters, 2015, 15, 3931-3938.	4.5	100

#	Article	IF	Citations
547	Interfacial Charge Transfer Anisotropy in Polycrystalline Lead Iodide Perovskite Films. Journal of Physical Chemistry Letters, 2015, 6, 1396-1402.	2.1	141
548	Unveiling the non-covalent interactions of molecular homodimers by dispersion-corrected DFT calculations and collision-induced broadening of ro-vibrational transitions: application to (CH2F2)2 and (SO2)2. Physical Chemistry Chemical Physics, 2015, 17, 5659-5669.	1.3	36
549	A benchmark database for adsorption bond energies to transition metal surfaces and comparison to selected DFT functionals. Surface Science, 2015, 640, 36-44.	0.8	396
550	Beyond Energies: Geometries of Nonbonded Molecular Complexes as Metrics for Assessing Electronic Structure Approaches. Journal of Chemical Theory and Computation, 2015, 11, 1481-1492.	2.3	90
551	Ab initio study of sodium intercalation into disordered carbon. Journal of Materials Chemistry A, 2015, 3, 9763-9768.	5.2	193
552	A first principles study of hydrogen storage on lithium decorated two dimensional carbon allotropes. International Journal of Hydrogen Energy, 2015, 40, 6128-6136.	3.8	53
553	A density functional study of silver clusters on a stepped graphite surface: formation of self-assembled nano-wires. Physical Chemistry Chemical Physics, 2015, 17, 12708-12716.	1.3	5
554	Short-Range Cut-Off of the Summed-Up van der Waals Series: Rare-Gas Dimers. Topics in Current Chemistry, 2015, , 53-80.	4.0	1
555	Identifying systematic DFT errors in catalytic reactions. Catalysis Science and Technology, 2015, 5, 4946-4949.	2.1	144
556	Toward a Database of Chemically Accurate Barrier Heights for Reactions of Molecules with Metal Surfaces. Journal of Physical Chemistry Letters, 2015, 6, 4106-4114.	2.1	67
557	Unexpected Photoreactivity in a NO₂-Functionalized Aluminum-MOF. Journal of Physical Chemistry C, 2015, 119, 26401-26408.	1.5	9
558	Nuclear Bound States of Molecular Hydrogen Physisorbed on Graphene: An Effective Two-Dimensional Model. Journal of Physical Chemistry A, 2015, 119, 11022-11032.	1.1	15
559	The Nature of the Interlayer Interaction in Bulk and Few-Layer Phosphorus. Nano Letters, 2015, 15, 8170-8175.	4.5	252
560	Molecular Self-Assembly in a Poorly Screened Environment: F₄TCNQ on Graphene/BN. ACS Nano, 2015, 9, 12168-12173.	7.3	45
561	Breaking Badly: DFT-D2 Gives Sizeable Errors for Tensile Strengths in Palladium-Hydride Solids. Journal of Chemical Theory and Computation, 2015, 11, 5426-5435.	2.3	74
562	First-Principles Study on Graphene/Hexagonal Boron Nitride Heterostructures. Journal of the Physical Society of Japan, 2015, 84, 121002.	0.7	21
563	Polymorphic, Porous, and Hostâ€“Guest Nanostructures Directed by Monolayerâ€“Substrate Interactions: Epitaxial Self-Assembly Study of Cyclic Trinuclear Au(I) Complexes on HOPG at the Solutionâ€“Solid Interface. Journal of Physical Chemistry C, 2015, 119, 24844-24858.	1.5	15
564	Ab initio calculations of optical constants of GaSe and InSe layered crystals. Physics of the Solid State, 2015, 57, 1735-1740.	0.2	7

#	Article	IF	Citations
565	Recent Advances in Two-Dimensional Materials beyond Graphene. ACS Nano, 2015, 9, 11509-11539.	7.3	2,069
566	A comparative chemisorption study of acrylic, vinyl acetic, fumaric, maleic and tartaric acid on Si(1 0) Tj ETQq1 1 0.784314 rgBT /Ove	1.1	5
567	Physisorbed H2@Cu(100) surface: Potential and spectroscopy. Journal of Chemical Physics, 2015, 142, 054703.	1.2	6
568	Communication: Water on hexagonal boron nitride from diffusion Monte Carlo. Journal of Chemical Physics, 2015, 142, 181101.	1.2	56
569	Coverage dependent work function of graphene on a Cu(111) substrate with intercalated alkali metals. Applied Physics Letters, 2015, 106, .	1.5	17
570	Non-pairwise additivity of the leading-order dispersion energy. Journal of Chemical Physics, 2015, 142, 084105.	1.2	1
571	Jump rates for surface diffusion of large molecules from first principles. Journal of Chemical Physics, 2015, 142, 154105.	1.2	1
572	Probing the mechanism of CO₂ capture in diamine-appended metalâ€“organic frameworks using measured and simulated X-ray spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 21448-21457.	1.3	43
573	Benzene derivatives adsorbed to the Ag(111) surface: Binding sites and electronic structure. Journal of Chemical Physics, 2015, 142, 101924.	1.2	22
574	The interactions between TiO₂ and graphene with surface inhomogeneity determined using density functional theory. Physical Chemistry Chemical Physics, 2015, 17, 29734-29746.	1.3	38
575	In-Plane Intermolecular Interaction Assisted Assembly and Modified Electronic States of Metallofullerene Gd@C₈₂. Langmuir, 2015, 31, 11438-11442.	1.6	3
576	DFT-based force field development for noble gas adsorption in metal organic frameworks. Journal of Materials Chemistry A, 2015, 3, 23539-23548.	5.2	33
577	Role of Long-Range Interactions for the Structure and Energetics of Olympicene Radical Adsorbed on Au(111) and Pt(111) Surfaces. Journal of Physical Chemistry C, 2015, 119, 25408-25419.	1.5	19
578	Benchmarking density functional theory predictions of framework structures and properties in a chemically diverse test set of metalâ€“organic frameworks. Journal of Materials Chemistry A, 2015, 3, 22432-22440.	5.2	64
579	Chemisorption of benzene on Pt (1 1 1) surface: A DFT study with van der Waals interaction. Chemical Physics Letters, 2015, 637, 182-188.	1.2	15
580	Performance of a Non-Local van der Waals Density Functional on the Dissociation of H₂ on Metal Surfaces. Journal of Physical Chemistry A, 2015, 119, 12146-12158.	1.1	44
581	Critical Factors Driving the High Volumetric Uptake of Methane in Cu₃(btc)₂. Journal of the American Chemical Society, 2015, 137, 10816-10825.	6.6	73
582	Effect of van der Waals interactions on the structural and binding properties of GaSe. Journal of Solid State Chemistry, 2015, 232, 67-72.	1.4	12

#	Article	IF	Citations
583	Anisotropic displacement parameters from dispersion-corrected DFT methods and their experimental validation by temperature-dependent X-ray diffraction. CrystEngComm, 2015, 17, 7414-7422.	1.3	27
584	Mechanistic insights into nitrogen fixation by nitrogenase enzymes. Physical Chemistry Chemical Physics, 2015, 17, 29541-29547.	1.3	84
585	Chemical accuracy from quantum Monte Carlo for the benzene dimer. Journal of Chemical Physics, 2015, 143, 104301.	1.2	19
586	Assessing the reliability of van der Waals DFT functionals to study the physisorption of molecular hydrogen on aromatic systems. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	6
587	Momentum microscopy of the layered semiconductor TiS₂and Ni intercalated Ni_{1/3}TiS₂. New Journal of Physics, 2015, 17, 083010.	1.2	23
588	Electrical Control of Spin States of Ferrocene on Cu(111). Journal of Physical Chemistry C, 2015, 119, 21681-21687.	1.5	15
589	Catalytic Role of the Substrate Defines Specificity of Therapeutic l-Asparaginase. Journal of Molecular Biology, 2015, 427, 2867-2885.	2.0	25
590	Measurement of the cleavage energy of graphite. Nature Communications, 2015, 6, 7853.	5.8	240
591	The Effect of Dispersion Correction on the Adsorption of CO on Metallic Nanoparticles. Journal of Physical Chemistry A, 2015, 119, 9703-9709.	1.1	60
592	Structural and electronic properties of crystalline graphite-like BC3. Computational Materials Science, 2015, 109, 248-252.	1.4	11
593	Local response dispersion method: A densityâ€dependent dispersion correction for density functional theory. International Journal of Quantum Chemistry, 2015, 115, 309-324.	1.0	12
594	Local response dispersion method in periodic systems: Implementation and assessment. Journal of Computational Chemistry, 2015, 36, 303-311.	1.5	4
595	First-principles insights into the nature of zirconiumâ€“iodine interactions and the initiation of iodine-induced stressâ€“corrosion cracking. Journal of Nuclear Materials, 2015, 458, 1-10.	1.3	18
596	Accurate, Precise, and Efficient Theoretical Methods To Calculate Anionâ”Ï€ Interaction Energies in Model Structures. Journal of Chemical Theory and Computation, 2015, 11, 360-371.	2.3	26
597	Current Understanding of Van der Waals Effects in Realistic Materials. Advanced Functional Materials, 2015, 25, 2054-2061.	7.8	101
598	Accurate Ab Initio Description of Adsorption on Coordinatively Unsaturated Cu2+ and Fe3+ Sites in MOFs. Journal of Chemical Theory and Computation, 2015, 11, 230-238.	2.3	36
599	Binding of nucleobases with graphene and carbon nanotube: a review of computational studies. Journal of Biomolecular Structure and Dynamics, 2015, 33, 1567-1597.	2.0	34
600	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561

#	Article	IF	Citations
601	Electronic Structure of ABC-stacked Multilayer Graphene and Trigonal Warping:A First Principles Calculation. Journal of Physics: Conference Series, 2016, 707, 012022.	0.3	7
602	Optical spectrum and excitons in bulk and monolayer MX2 (M=Zr, Hf; X=S, Se). Physica Status Solidi (B): Basic Research, 2016, 253, 705-711.	0.7	32
603	Electronic and optical properties of MX₃ (M = Ti, Zr and Hf; X = S, Se) structures: A first principles insight. Physica Status Solidi (B): Basic Research, 2016, 253, 868-874.	0.7	17
604	Dynamic Entangled Porous Framework for Hydrocarbon (C2â€“C3) Storage, CO₂ Capture, and Separation. Chemistry - A European Journal, 2016, 22, 6059-6070.	1.7	48
605	CO₂ Capture in Aluminumâ€Based Metalâ€organic Frameworks: A Theoretical Study. Journal of the Chinese Chemical Society, 2016, 63, 459-464.	0.8	4
606	A Theoretical Study on the Design, Structure, and Electronic Properties of Novel Forms of Graphynes. Journal of Physical Chemistry C, 2016, 120, 15153-15161.	1.5	54
608	Quantifying Uncertainty in Activity Volcano Relationships for Oxygen Reduction Reaction. ACS Catalysis, 2016, 6, 5251-5259.	5.5	70
609	Modeling surface motion effects in N2 dissociation on W(110): Ab initio molecular dynamics calculations and generalized Langevin oscillator model. Journal of Chemical Physics, 2016, 144, 244708.	1.2	19
610	Interplay of Chemical and Electronic Structure on the Single-Molecule Level in 2D Polymerization. ACS Nano, 2016, 10, 11511-11518.	7.3	35
611	The atomic structures and electronic properties of potassium-doped phenanthrene from a first-principles study. Journal of Materials Chemistry C, 2016, 4, 11566-11571.	2.7	11
612	First-principles study of the pressure effects on the structural and electronic properties of crystalline organic azide C10H8N6O4. Journal of Structural Chemistry, 2016, 57, 1074-1078.	0.3	2
613	Self-consistent implementation of meta-GGA functionals for the ONETEP linear-scaling electronic structure package. Journal of Chemical Physics, 2016, 145, 204114.	1.2	18
614	Methane dissociation on Pt(111): Searching for a specific reaction parameter density functional. Journal of Chemical Physics, 2016, 144, 044702.	1.2	52
615	Lattice thermal expansion and anisotropic displacements in ?-sulfur from diffraction experiments and first-principles theory. Journal of Chemical Physics, 2016, 145, 234512.	1.2	19
616	Application of van der Waals functionals to the calculation of dissociative adsorption of N2 on W(110) for static and dynamic systems. Journal of Chemical Physics, 2016, 144, 084702.	1.2	12
617	Effect of van der Waals interactions on the chemisorption and physisorption of phenol and phenoxy on metal surfaces. Journal of Chemical Physics, 2016, 145, 104701.	1.2	21
618	On the tautomerisation of porphycene on copper (111): Finding the subtle balance between van der Waals interactions and hybridisation. Journal of Chemical Physics, 2016, 145, 244701.	1.2	5
619	Discriminating between Metallic and Semiconducting Single-Walled Carbon Nanotubes Using Physisorbed Adsorbates: Role of Wavelike Charge-Density Fluctuations. Physical Review Letters, 2016, 117, 246101.	2.9	16

#	Article	IF	Citations
620	The dynamics of copper intercalated molybdenum ditelluride. Journal of Chemical Physics, 2016, 145, 194702.	1.2	8
621	Density-functional description of polymer crystals: A comparative study of recent van der Waals functionals. Journal of Chemical Physics, 2016, 144, 214905.	1.2	12
622	Rungs 1 to 4 of DFT Jacobâ€™s ladder: Extensive test on the lattice constant, bulk modulus, and cohesive energy of solids. Journal of Chemical Physics, 2016, 144, 204120.	1.2	191
623	First-principles study on equation of states and electronic structures of shock compressed Ar up to warm dense regime. Journal of Chemical Physics, 2016, 144, 124503.	1.2	14
624	Blind test of density-functional-based methods on intermolecular interaction energies. Journal of Chemical Physics, 2016, 145, 124105.	1.2	97
625	Low-pressure phase diagram of crystalline benzene from quantum Monte Carlo. Journal of Chemical Physics, 2016, 145, .	1.2	11
626	Perspective: Kohn-Sham density functional theory descending a staircase. Journal of Chemical Physics, 2016, 145, 130901.	1.2	243
627	First-principles Hubbard U approach for small molecule binding in metal-organic frameworks. Journal of Chemical Physics, 2016, 144, 174104.	1.2	73
628	Perspective: How good is DFT for water?. Journal of Chemical Physics, 2016, 144, 130901.	1.2	571
629	Influence of the exchange and correlation functional on the structure of amorphous InSb and In3SbTe2 compounds. Journal of Chemical Physics, 2016, 144, 204508.	1.2	8
630	Physisorption mechanism in graphene/noble metal (111)/Ni(111) heterostructures: An ab-initio study. Journal of Applied Physics, 2016, 120, 075301.	1.1	1
631	Note: The performance of new density functionals for a recent blind test of non-covalent interactions. Journal of Chemical Physics, 2016, 145, 186101.	1.2	11
632	Structure and dynamics of aqueous solutions from PBE-based first-principles molecular dynamics simulations. Journal of Chemical Physics, 2016, 145, 154501.	1.2	87
633	Surface tension of ab initio liquid water at the water-air interface. Journal of Chemical Physics, 2016, 144, 204705.	1.2	39
634	Ï‰B97M-V: A combinatorially optimized, range-separated hybrid, meta-GGA density functional with VV10 nonlocal correlation. Journal of Chemical Physics, 2016, 144, 214110.	1.2	595
635	Post-Hartree-Fock studies of the He/Mg(0001) interaction: Anti-corrugation, screening, and pairwise additivity. Journal of Chemical Physics, 2016, 144, 244707.	1.2	16
636	A polymer dataset for accelerated property prediction and design. Scientific Data, 2016, 3, 160012.	2.4	139
637	Approaching the basis set limit for DFT calculations using an environment-adapted minimal basis with perturbation theory: Formulation, proof of concept, and a pilot implementation. Journal of Chemical Physics, 2016, 145, 044109.	1.2	16

#	Article	IF	Citations
638	Molecular spin on surface: From strong correlation to dispersion interactions. Journal of Chemical Physics, 2016, 145, 124704.	1.2	9
639	From small fullerenes to the graphene limit: A harmonic forceâ€field method for fullerenes and a comparison to density functional calculations for <scp>G</scp>oldbergâ€“<scp>C</scp>oxeter fullerenes up to C₉₈₀. Journal of Computational Chemistry, 2016, 37, 10-17.	1.5	12
640	Recent development of atomâ€pairwise van der waals corrections for density functional theory: From molecules to solids. International Journal of Quantum Chemistry, 2016, 116, 598-607.	1.0	19
641	Modulating Bond Lengths via Backdonation: A First-Principles Investigation of a Quinonoid Zwitterion Adsorbed to Coinage Metal Surfaces. Journal of Physical Chemistry C, 2016, 120, 6633-6641.	1.5	11
642	Optical Properties of Gold Nanoclusters Functionalized with a Small Organic Compound: Modeling by an Integrated Quantum-Classical Approach. Journal of Chemical Theory and Computation, 2016, 12, 3325-3339.	2.3	9
643	An ab initio molecular dynamics study of D2 dissociation on CO-precovered Ru(0001). Physical Chemistry Chemical Physics, 2016, 18, 21190-21201.	1.3	3
644	Force Field Development from Periodic Density Functional Theory Calculations for Gas Separation Applications Using Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2016, 120, 12590-12604.	1.5	95
645	Quantitative Understanding of van der Waals Interactions by Analyzing the Adsorption Structure and Low-Frequency Vibrational Modes of Single Benzene Molecules on Silver. Journal of Physical Chemistry Letters, 2016, 7, 2228-2233.	2.1	6
646	Modeling and simulation of proteinâ€“surface interactions: achievements and challenges. Quarterly Reviews of Biophysics, 2016, 49, e4.	2.4	163
647	Screened exchange hybrid density functional for accurate and efficient structures and interaction energies. Physical Chemistry Chemical Physics, 2016, 18, 15519-15523.	1.3	49
648	The interaction of Pd clusters with the bulk and layered two-dimensional Silicalite-1 supports. Catalysis Today, 2016, 277, 108-117.	2.2	2
649	Adsorption and electronic properties of Fullerene/Zn-Phthalocyanine (C60/ZnPc) interface with face-on orientation: A van der Waals corrected Density Functional Theory investigation. Chemical Physics Letters, 2016, 649, 73-77.	1.2	9
650	Thermodynamics of gas adsorption in <scp>MOF</scp>s using Ab Initio calculations. International Journal of Quantum Chemistry, 2016, 116, 569-572.	1.0	9
651	Dispersion-Corrected Mean-Field Electronic Structure Methods. Chemical Reviews, 2016, 116, 5105-5154.	23.0	1,032
652	The role of vdW interactions in coverage dependent adsorption energies of atomic adsorbates on Pt(111) and Pd(111). Surface Science, 2016, 650, 196-202.	0.8	5
653	Van Der Waals-Corrected Density Functional Theory Simulation of Adsorption Processes on Noble-Metal Surfaces: Xe on Ag(111), Au(111), and Cu(111). Journal of Low Temperature Physics, 2016, 185, 183-197.	0.6	13
654	Structural Evolution of Reversible Mg Insertion into a Bilayer Structure of V₂O₅Â·nH₂O Xerogel Material. Chemistry of Materials, 2016, 28, 2962-2969.	3.2	97
655	A van der Waals Density Functional Study of MoO₃ and Its Oxygen Vacancies. Journal of Physical Chemistry C, 2016, 120, 8959-8968.	1.5	91

#	Article	IF	Citations
656	Modeling the Interface of Platinum and Î±-Quartz(001): Implications for Sintering. Journal of Physical Chemistry C, 2016, 120, 10340-10350.	1.5	18
657	A Series of Layered Assemblies of Hydrogen-Bonded, Hexagonal Networks of C₃-Symmetric Ï€-Conjugated Molecules: A Potential Motif of Porous Organic Materials. Journal of the American Chemical Society, 2016, 138, 6617-6628.	6.6	169
658	Interaction of boron with graphite: A van der Waals density functional study. Applied Surface Science, 2016, 379, 402-410.	3.1	15
659	Hydrostatic Pressure Effects on Structural and Electronic Properties of ETN and PETN from First-Principles Calculations. Journal of Physical Chemistry A, 2016, 120, 3710-3717.	1.1	8
660	The Effect of the Electric Field on the Î±-GPC Interaction with Au(111) Surface: A First-Principles Study. Journal of Physical Chemistry C, 2016, 120, 9740-9749.	1.5	2
661	Density Functional Theory Methods for Computing and Predicting Mechanical Properties. Springer Series in Materials Science, 2016, , 131-158.	0.4	0
662	Organic crystal polymorphism: a benchmark for dispersion-corrected mean-field electronic structure methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 502-513.	0.5	53
663	Hydrogen adsorption on Li-decorated BN analogs of Î³-graphyne: A DFT study. Computational Materials Science, 2016, 125, 28-35.	1.4	29
664	Theoretical study of disorder-order transition of sodium borohydride. Computational Materials Science, 2016, 124, 87-91.	1.4	3
665	Magnetic and Electronic Properties of Samarium-Doped Phenanthrene from First-Principles Study. Journal of Physical Chemistry C, 2016, 120, 22565-22570.	1.5	12
666	Layer-dependent properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="bold">SnS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="bold">SnSe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>two-dimensional materials. Physical Review B, 2016, 94, .	1.1	267
667	Probing gas adsorption in MOFs using an efficient ab initio widom insertion Monte Carlo method. Journal of Computational Chemistry, 2016, 37, 2808-2815.	1.5	8
668	Screening of Copper Open Metal Site MOFs for Olefin/Paraffin Separations Using DFT-Derived Force Fields. Journal of Physical Chemistry C, 2016, 120, 23044-23054.	1.5	61
669	A new 2D monolayer BiXene, M₂C (M = Mo, Tc, Os). Nanoscale, 2016, 8, 15753-15762.	2.8	46
670	van der Waals density functionals applied to corundum-type sesquioxides: bulk properties and adsorption of CH₃ and C₆H₆ on (0001) surfaces. Physical Chemistry Chemical Physics, 2016, 18, 23139-23146.	1.3	7
671	Calcium decorated two dimensional carbon allotropes for hydrogen storage: A first-principles study. Computational Materials Science, 2016, 124, 106-113.	1.4	25
672	Electronic Structure of the (Undoped and Fe-Doped) NiOOH O₂ Evolution Electrocatalyst. Journal of Physical Chemistry C, 2016, 120, 18999-19010.	1.5	52
674	Immobilization of Au nanoparticles on graphite tunnels through nanocapillarity. RSC Advances, 2016, 6, 77195-77200.	1.7	12

#	Article	IF	Citations
675	Structural Studies of Polyaramid Fibers: Solid-State NMR and First-Principles Modeling. Macromolecules, 2016, 49, 5548-5560.	2.2	12
676	Cohesive properties of noble metals by van der Waalsâ€“corrected density functional theory: Au, Ag, and Cu as case studies. Physical Review B, 2016, 94, .	1.1	28
677	Adsorption of Noble-Gas Atoms on the TiO₂(110) Surface: An Ab Initio-Assisted Study with van der Waals-Corrected DFT. Journal of Physical Chemistry C, 2016, 120, 18126-18139.	1.5	51
678	Electronic Band Structure of 2D TMDCs. Springer Series in Materials Science, 2016, , 165-226.	0.4	1
679	van der Waals effects on grazing-incidence fast-atom diffraction for H on LiF(001). Physical Review A, 2016, 94, .	1.0	15
680	High-capacity hydrogen storage in Li-adsorbed g-C3N4. Materials Chemistry and Physics, 2016, 180, 440-444.	2.0	21
681	A Quasi-Free-Standing Single Layer of a B3N3-Doped Nanographene Molecule Deposited on Au(111) Single Crystals. Journal of Physical Chemistry C, 2016, 120, 17645-17651.	1.5	14
682	Adsorption in zeolites using mechanically embedded ONIOM clusters. Physical Chemistry Chemical Physics, 2016, 18, 26094-26106.	1.3	35
683	Kineticâ€energyâ€density dependent semilocal exchangeâ€correlation functionals. International Journal of Quantum Chemistry, 2016, 116, 1641-1694.	1.0	78
684	A van der Waals density functional theory study of poly(vinylidene difluoride) crystallineÂphases. European Physical Journal: Special Topics, 2016, 225, 1733-1742.	1.2	5
685	Chromate adsorption mechanism on nanodiamond-derived onion-like carbon. Journal of Hazardous Materials, 2016, 320, 368-375.	6.5	25
686	Capturing Solvation Effects at a Liquid/Nanoparticle Interface by Ab Initio Molecular Dynamics: Pt₂₀₁ Immersed in Water. Small, 2016, 12, 5312-5319.	5.2	25
687	Lithium Ion Disorder and Conduction Mechanism in LiCe(BH₄)₃Cl. Journal of Physical Chemistry C, 2016, 120, 19035-19042.	1.5	20
688	Germanene: a new electronic gas sensing material. RSC Advances, 2016, 6, 102264-102271.	1.7	68
689	Binary functionalization of H:Si(111) surfaces by alkyl monolayers with different linker atoms enhances monolayer stability and packing. Physical Chemistry Chemical Physics, 2016, 18, 12952-12963.	1.3	5
690	Surface directed reversible imidazole ligation to nickel(<scp>ii</scp>) octaethylporphyrin at the solution/solid interface: a single molecule level study. Physical Chemistry Chemical Physics, 2016, 18, 20819-20829.	1.3	23
691	Toward More Complete Descriptors of Reactivity in Catalysis by Solid Acids. ACS Catalysis, 2016, 6, 5386-5392.	5.5	42
692	Solid state synthesis, structural characterization and ionic conductivity of bimetallic alkali-metal yttrium borohydrides MY(BH₄)₄ (M = Li and Na). Journal of Materials Chemistry A, 2016, 4, 8793-8802.	5.2	37

#	Article	IF	Citations
693	Role of van der Waals forces in the diffraction of noble gases from metal surfaces. Physical Review B, 2016, 93, .	1.1	21
694	Dual role of Fe dopants in enhancing stability and charge transfer in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>(</mml:mo><mml:msub><mml:mi>Li</mml:mi></mml:msub><mml:mi> Physical Review B, 2016, 93, .	1.1	15
695	Structural and excited-state properties of oligoacene crystals from first principles. Physical Review B, 2016, 93, .	1.1	89
696	Ab initiostudy of the one-dimensional H-bonded ferroelectricCsH2PO4. Physical Review B, 2016, 93, .	1.1	17
697	Interatomic force constants including the DFT-D dispersion contribution. Physical Review B, 2016, 93, .	1.1	50
698	Crystal structure and magnetism in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î±</mml:mi><mml:mo>â^'</mml:mo><mml:msub><mml:mi> Anab initiostudy. Physical Review B, 2016, 93, .	1.1	104
699	Molecular bonding with the RPAx: From weak dispersion forces to strong correlation. Physical Review B, 2016, 93, .	1.1	18
700	Ab initiophonon dispersion in crystalline naphthalene using van der Waals density functionals. Physical Review B, 2016, 93, .	1.1	41
701	Exchange interactions of magnetic surfaces below two-dimensional materials. Physical Review B, 2016, 93, .	1.1	8
702	Dislocations in stacking and commensurate-incommensurate phase transition in bilayer graphene and hexagonal boron nitride. Physical Review B, 2016, 93, .	1.1	28
703	Self-consistent van der Waals density functional study of benzene adsorption on Si(100). Physical Review B, 2016, 93, .	1.1	45
704	Binding energies of nucleobase complexes: Relevance to homology recognition of DNA. Physical Review E, 2016, 93, 062410.	0.8	3
705	Probing Carrier Transport and Structure-Property Relationship of Highly Ordered Organic Semiconductors at the Two-Dimensional Limit. Physical Review Letters, 2016, 116, 016602.	2.9	220
706	Graphene nanoribbons anchored to SiC substrates. Journal of Physics Condensed Matter, 2016, 28, 364001.	0.7	2
707	Structural, Dynamical, and Electronic Properties of Liquid Water: A Hybrid Functional Study. Journal of Physical Chemistry B, 2016, 120, 7456-7470.	1.2	61
708	Density-functional theory with screened van der Waals interactions applied to atomic and molecular adsorbates on close-packed and non-close-packed surfaces. Physical Review B, 2016, 93, .	1.1	90
709	Benchmarking density functionals for hydrogen-helium mixtures with quantum Monte Carlo: Energetics, pressures, and forces. Physical Review B, 2016, 93, .	1.1	34
710	Layered structures of organic/inorganic hybrid halide perovskites. Physical Review B, 2016, 93, .	1.1	31

#	Article	IF	Citations
711	Energy level alignment of self-assembled linear chains of benzenediamine on Au(111) from first principles. Physical Review B, 2016, 93, .	1.1	8
712	Phonons in nonlocal van der Waals density functional theory. Physical Review B, 2016, 93, .	1.1	17
713	mBEEF-vdW: Robust fitting of error estimation density functionals. Physical Review B, 2016, 93, .	1.1	35
714	Proposal for a bulk material based on a monolayer FeSe on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><m superconductor. Physical Review B, 2016, 93, .	1.1	10
715	Structure and Growth of Hexagonal Boron Nitride on Ir(111). ACS Nano, 2016, 10, 11012-11026.	7.3	93
716	Assessing the influence of van der Waals corrected exchange-correlation functionals on the anisotropic mechanical properties of coinage metals. Physical Review B, 2016, 94, .	1.1	19
717	Descriptors and Thermodynamic Limitations of Electrocatalytic Carbon Dioxide Reduction on Rutile Oxide Surfaces. ChemSusChem, 2016, 9, 3230-3243.	3.6	34
718	Interaction of Black Phosphorus with Oxygen and Water. Chemistry of Materials, 2016, 28, 8330-8339.	3.2	436
719	A Combined Energy-Force Fitting Procedure to Develop DFT-Based Force Fields. Journal of Physical Chemistry C, 2016, 120, 26309-26319.	1.5	3
720	First-principles studies of electric field effects on the electronic structure of trilayer graphene. Physical Review B, 2016, 94, .	1.1	20
721	Comprehensive structureâ€“function correlation of photoactive ionic Ï€-conjugated supermolecular assemblies: an experimental and computational study. Journal of Materials Chemistry C, 2016, 4, 10223-10239.	2.7	32
722	Versatile van der Waals Density Functional Based on a Meta-Generalized Gradient Approximation. Physical Review X, 2016, 6, .	2.8	321
723	Observation of Nanoscale Morphological and Structural Degradation in Perovskite Solar Cells by in Situ TEM. ACS Applied Materials & Interfaces, 2016, 8, 32333-32340.	4.0	54
724	Promoting Atoms into Delocalized Long-Living Magnetically Modified State Using Atomic Force Microscopy. Nano Letters, 2016, 16, 7490-7494.	4.5	2
725	Electronic Properties of Homo- and Heterobilayer Graphyne: The Idea of a Nanocapacitor. Journal of Physical Chemistry C, 2016, 120, 26579-26587.	1.5	57
726	Nitrogen induced phosphorene formation on the boron phosphide (111) surface: a density functional theory study. RSC Advances, 2016, 6, 108621-108626.	1.7	2
727	Functional Independent Scaling Relation for ORR/OER Catalysts. Journal of Physical Chemistry C, 2016, 120, 24910-24916.	1.5	119
728	Ditechnetium Heptoxide Revisited: Solid-State, Gas-Phase, and Theoretical Studies. Inorganic Chemistry, 2016, 55, 10445-10452.	1.9	17

#	Article	IF	Citations
730	Dioxin sensing properties of graphene and hexagonal boron nitride based van der Waals solids: a first-principles study. RSC Advances, 2016, 6, 107114-107126.	1.7	5
731	Halogenâ^Ï€ Interactions between Benzene and X2/CX4 (X = Cl, Br): Assessment of Various Density Functionals with Respect to CCSD(T). Journal of Physical Chemistry A, 2016, 120, 9305-9314.	1.1	32
732	Toward Accurate Adsorption Energetics on Clay Surfaces. Journal of Physical Chemistry C, 2016, 120, 26402-26413.	1.5	30
733	Structural, electronic and kinetic properties of the phase-change material Ge2Sb2Te5 in the liquid state. Scientific Reports, 2016, 6, 27434.	1.6	37
734	Materials perspective on Casimir and van der Waals interactions. Reviews of Modern Physics, 2016, 88, .	16.4	276
735	Nuclear and Electron Wave Packet Molecular Dynamics Simulation Method and Its Application to Liquid, Solid and Supercooled Hydrogens. Molecular Science, 2016, 10, A0084.	0.2	0
736	Anomalous bond length behavior and a new solid phase of bromine under pressure. Scientific Reports, 2016, 6, 25649.	1.6	13
737	van der Waals potential energy surfaces from the exchange-hole dipole moment dispersion model. Canadian Journal of Chemistry, 2016, 94, 1049-1056.	0.6	1
738	Combined experimental and computational study of high-pressure behavior of triphenylene. Scientific Reports, 2016, 6, 25600.	1.6	12
739	Insights into the spurious long-range nature of local rs-dependent non-local exchange-correlation kernels. Journal of Chemical Physics, 2016, 145, 054121.	1.2	0
740	In silico engineering of grapheneâ€based van der Waals heterostructured nanohybrids for electronics and energy applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 551-570.	6.2	32
741	Theoretical Studies of Oxygen Reactivity of Freeâ€Standing and Supported Boronâ€Doped Graphene. ChemSusChem, 2016, 9, 1061-1077.	3.6	12
742	Density functional theory study of interaction of graphene with hypoxanthine, xanthine, and uric acid. Molecular Physics, 2016, 114, 2157-2163.	0.8	21
743	Structural Evolution of Solid Phenanthrene at High Pressures. Journal of Physical Chemistry C, 2016, 120, 14310-14316.	1.5	11
744	A density functional theory study for the adsorption of various gases on a caesium-exchanged trapdoor chabazite. Computational Materials Science, 2016, 122, 307-313.	1.4	25
745	Structural and electronic properties of solid naphthalene under pressure: density functional calculations. European Physical Journal B, 2016, 89, 1.	0.6	5
746	Unraveling the Intercalation Chemistry of Hexagonal Tungsten Bronze and Its Optical Responses. Chemistry of Materials, 2016, 28, 4528-4535.	3.2	47
747	Exchangeâ€“Correlation Effects for Noncovalent Interactions in Density Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 3160-3175.	2.3	24

#	Article	IF	Citations
748	Molecular dynamics and first-principles studies of structural change in 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) in crystalline state under high pressure: Comparison of hydrogen bond systems of TATB versus 1,3-diamino-2,4,6-trinitrobenzene (DATB). Chemical Physics, 2016, 472, 163-172.	0.9	19
749	H/He demixing and the cooling behavior of Saturn. Icarus, 2016, 267, 323-333.	1.1	26
750	Effects of Chain Length on the Mechanism and Rates of Metal-Catalyzed Hydrogenolysis of n-Alkanes. Journal of Physical Chemistry C, 2016, 120, 8125-8138.	1.5	49
751	Vapor Liquid Equilibria of Hydrofluorocarbons Using Dispersion-Corrected and Nonlocal Density Functionals. Journal of Chemical Theory and Computation, 2016, 12, 3295-3304.	2.3	11
752	NMR study and computational assays of meclofenamic Na salt and Î²-cyclodextrin inclusion complex. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 85, 111-120.	0.9	7
753	How theory and simulation can drive fuel cell electrocatalysis. Nano Energy, 2016, 29, 334-361.	8.2	71
754	Surface Adsorption from the Exchange-Hole Dipole Moment Dispersion Model. Journal of Chemical Theory and Computation, 2016, 12, 3305-3315.	2.3	43
755	Effects of an electric field on interaction of aromatic systems. Journal of Computational Chemistry, 2016, 37, 971-975.	1.5	7
756	Problems, successes and challenges for the application of dispersion-corrected density-functional theory combined with dispersion-based implicit solvent models to large-scale hydrophobic self-assembly and polymorphism. Molecular Simulation, 2016, 42, 494-510.	0.9	13
757	Theoretical Study of Trimethylacetic Acid Adsorption on CeO₂(111) Surface. Journal of Physical Chemistry C, 2016, 120, 2655-2666.	1.5	12
758	Theoretical study of the interactions of a graphene-on-Ni(111) composite with dopamine. Molecular Physics, 2016, 114, 829-834.	0.8	3
759	Phase diagrams for clathrate hydrates of methane, ethane, and propane from first-principles thermodynamics. Physical Chemistry Chemical Physics, 2016, 18, 3272-3279.	1.3	15
760	Stacking-Mode-Induced Reactivity Enhancement for Twisted Bilayer Graphene. Chemistry of Materials, 2016, 28, 1034-1039.	3.2	35
761	Anisotropy in lattice thermal conductivity tensor of bulk hexagonal-MT₂ (M = W, Mo and) Tj ETQq1 1 0.784314 rgBT /Over	1.7	15
762	Toward an Accurate Estimate of the Exfoliation Energy of Black Phosphorus: A Periodic Quantum Chemical Approach. Journal of Physical Chemistry Letters, 2016, 7, 131-136.	2.1	62
763	Interlayer interaction and related properties of bilayer hexagonal boron nitride: ab initio study. RSC Advances, 2016, 6, 6423-6435.	1.7	37
764	Role of Structural H₂O in Intercalation Electrodes: The Case of Mg in Nanocrystalline Xerogel-V₂O₅. Nano Letters, 2016, 16, 2426-2431.	4.5	194
765	Polytypism and unexpected strong interlayer coupling in two-dimensional layered ReS₂. Nanoscale, 2016, 8, 8324-8332.	2.8	120

#	Article	IF	Citations
766	Structure and electronic properties of C₂N/graphene predicted by first-principles calculations. RSC Advances, 2016, 6, 28484-28488.	1.7	56
767	Mixed Valence Tin Oxides as Novel van der Waals Materials: Theoretical Predictions and Potential Applications. Advanced Energy Materials, 2016, 6, 1501190.	10.2	79
768	How strong is the edge effect in the adsorption of anticancer drugs on a graphene cluster?. Journal of Molecular Modeling, 2016, 22, 85.	0.8	14
769	Modeling Polymorphic Molecular Crystals with Electronic Structure Theory. Chemical Reviews, 2016, 116, 5567-5613.	23.0	294
770	Two-dimensional interlocked pentagonal bilayer ice: how do water molecules form a hydrogen bonding network?. Physical Chemistry Chemical Physics, 2016, 18, 14216-14221.	1.3	26
771	Interface-Induced Renormalization of Electrolyte Energy Levels in Magnesium Batteries. Journal of Physical Chemistry Letters, 2016, 7, 874-881.	2.1	39
772	A new phase diagram of water under negative pressure: The rise of the lowest-density clathrate s-III. Science Advances, 2016, 2, e1501010.	4.7	92
773	Interlayer Interactions in van der Waals Heterostructures: Electron and Phonon Properties. ACS Applied Materials & Interfaces, 2016, 8, 6286-6292.	4.0	63
774	Preferential activation of CO near hydrocarbon chains during Fischerâ€“Tropsch synthesis on Ru. Journal of Catalysis, 2016, 337, 91-101.	3.1	54
775	Synthesis of Atomically Precise Graphene-Based Nanostructures: A Simulation Point of View. Advances in Atom and Single Molecule Machines, 2016, , 237-268.	0.0	5
776	Structural, electronic and optical properties of TcX2 (X = S, Se, Te) from first principles calculations. Computational Materials Science, 2016, 115, 177-183.	1.4	18
777	Intrinsic Selectivity and Structure Sensitivity of Rhodium Catalysts for C₂₊ Oxygenate Production. Journal of the American Chemical Society, 2016, 138, 3705-3714.	6.6	179
778	First-Principles Study of the Structural, Electronic, Dynamic, and Mechanical Properties of HOPG and Diamond: Influence of Exchangeâ€“Correlation Functionals and Dispersion Interactions. Journal of Physical Chemistry C, 2016, 120, 5083-5100.	1.5	23
779	Theoretical Studies of Functionalised Silicene. Springer Series in Materials Science, 2016, , 107-127.	0.4	1
780	Computational Assessment of the Dominant Factors Governing the Mechanism of Methanol Dehydration over H-ZSM-5 with Heterogeneous Aluminum Distribution. ACS Catalysis, 2016, 6, 2287-2298.	5.5	92
781	First-principles study on the adsorption and dissociation of H2 molecules on Be(0 0 0 1) surfaces. Computational Materials Science, 2016, 117, 251-258.	1.4	6
782	Stabilizing and Modulating Color by Copigmentation: Insights from Theory and Experiment. Chemical Reviews, 2016, 116, 4937-4982.	23.0	408
783	Lithium diffusion in graphene and graphite: Effect of edge morphology. Carbon, 2016, 103, 209-216.	5.4	53

#	Article	IF	Citations
784	NO adsorption on Cu(110) and O(2 Ã— 1)/Cu(110) surfaces from density functional theory calculations. Physical Chemistry Chemical Physics, 2016, 18, 9476-9483.	1.3	8
785	Thermodynamic Properties of Molecular Crystals Calculated within the Quasi-Harmonic Approximation. Journal of Physical Chemistry A, 2016, 120, 2022-2034.	1.1	48
786	Combinations of coupled cluster, density functionals, and the random phase approximation for describing static and dynamic correlation, and van der Waals interactions. Molecular Physics, 2016, 114, 997-1018.	0.8	23
787	Lifshitz transition and modulation of electronic and transport properties of bilayer graphene by sliding and applied normal compressive strain. Carbon, 2016, 99, 432-438.	5.4	22
788	Interlayer electronic hybridization leads to exceptional thickness-dependent vibrational properties in few-layer black phosphorus. Nanoscale, 2016, 8, 2740-2750.	2.8	153
789	The pressure induced twisted distortion in the flexible oxide Tc2O7. CrystEngComm, 2016, 18, 328-333.	1.3	5
790	Scaling Relationships for Binding Energies of Transition Metal Complexes. Catalysis Letters, 2016, 146, 304-308.	1.4	25
791	Silver(i), gold(i) and palladium(ii) complexes of a NHC-pincer ligand with an aminotriazine core: a comparison with pyridyl analogues. Dalton Transactions, 2016, 45, 1484-1495.	1.6	15
792	Charge injection barriers at metal/polyethylene interfaces. Journal of Materials Science, 2016, 51, 506-512.	1.7	56
793	Geometry and Electronic Properties of Glycerol Adsorbed on Bare and Transition-Metal Surface-Alloyed Au(111): A Density Functional Theory Study. Journal of Physical Chemistry C, 2016, 120, 1749-1757.	1.5	18
794	Ethene Oligomerization in Ni-Containing Zeolites: Theoretical Discrimination of Reaction Mechanisms. ACS Catalysis, 2016, 6, 1205-1214.	5.5	106
795	Analytical nuclear gradients for the range-separated many-body dispersion model of noncovalent interactions. Chemical Science, 2016, 7, 1712-1728.	3.7	33
796	Oxygen orders differently under graphene: new superstructures on Ir(111). Nanoscale, 2016, 8, 1932-1943.	2.8	25
797	First principles study of enhanced CO 2 adsorption on MOF-253 by salt-insertion. Computational Materials Science, 2016, 111, 79-85.	1.4	7
798	Noncovalent Intermolecular Interactions in Organic Electronic Materials: Implications for the Molecular Packing vs Electronic Properties of Acenes. Chemistry of Materials, 2016, 28, 3-16.	3.2	215
799	Computational Chemistry of Catalytic Biomass Conversion. Green Chemistry and Sustainable Technology, 2016, , 63-104.	0.4	0
800	Effect of nitrogen doping on titanium carbonitride-derived adsorbents used for arsenic removal. Journal of Hazardous Materials, 2016, 302, 375-385.	6.5	24
801	Modelling of graphene functionalization. Physical Chemistry Chemical Physics, 2016, 18, 6351-6372.	1.3	190

#	Article	IF	Citations
802	First-principles study of two-dimensional van der Waals heterojunctions. Computational Materials Science, 2016, 112, 518-526.	1.4	88
803	Quantum and classical dynamics of reactive scattering of H₂ from metal surfaces. Chemical Society Reviews, 2016, 45, 3658-3700.	18.7	137
804	Giant Anisotropic Raman Response of Encapsulated Ultrathin Black Phosphorus by Uniaxial Strain. Advanced Functional Materials, 2017, 27, 1600986.	7.8	100
805	Influence of Surface Termination on the Energy Level Alignment at the CH₃NH₃PbI₃ Perovskite/C60 Interface. Chemistry of Materials, 2017, 29, 958-968.	3.2	149
806	Epitaxy-Induced Assembly and Enantiomeric Switching of an On-Surface Formed Dinuclear Organocobalt Complex. ACS Nano, 2017, 11, 1347-1359.	7.3	8
807	Long-range interactions from the many-pair expansion: A different avenue to dispersion in DFT. Journal of Chemical Physics, 2017, 146, 024111.	1.2	6
808	Prediction of a new ice clathrate with record low density: A potential candidate as ice XIX in guest-free form. Chemical Physics Letters, 2017, 671, 186-191.	1.2	36
809	AcceleratingabÂinitioMolecular Dynamics and Probing the Weak Dispersive Forces in Dense Liquid Hydrogen. Physical Review Letters, 2017, 118, 015703.	2.9	23
810	Comments on â€œGeometry and fast diffusion of AlCl 4 cluster intercalated in graphite [Electrochim. Acta 195 (2016) 158â€“165]â€• Electrochimica Acta, 2017, 223, 135-136.	2.6	16
811	Structural and electronic properties of potassium-doped 1,2;8,9-dibenzopentacene superconductor: comparing with doped [7]phenacenes. Molecular Physics, 2017, 115, 472-483.	0.8	18
812	Chemically accurate simulation of dissociative chemisorption of D2 on Pt(1 1 1). Chemical Physics Letters, 2017, 683, 329-335.	1.2	37
813	Adsorption of Organic Molecules to van der Waals Materials: Comparison of Fluorographene and Fluorographite with Graphene and Graphite. Journal of Chemical Theory and Computation, 2017, 13, 1328-1340.	2.3	47
814	A New Type of Scaling Relations to Assess the Accuracy of Computational Predictions of Catalytic Activities Applied to the Oxygen Evolution Reaction. ChemCatChem, 2017, 9, 1261-1268.	1.8	75
815	First-principles prediction on geometrical and electronic properties of K-doped chrysene. Journal of Physics and Chemistry of Solids, 2017, 104, 56-61.	1.9	14
816	Elementary steps in acetone condensation reactions catalyzed by aluminosilicates with diverse void structures. Journal of Catalysis, 2017, 346, 134-153.	3.1	73
817	Engineering of the interactions of volatile organic compounds with MoS₂. Journal of Materials Chemistry C, 2017, 5, 1463-1470.	2.7	30
818	Adsorption of CO₂ on Graphene: A Combined TPD, XPS, and vdW-DF Study. Journal of Physical Chemistry C, 2017, 121, 2807-2814.	1.5	76
819	Sodium-Induced Reordering of Atomic Stacks in Black Phosphorus. Chemistry of Materials, 2017, 29, 1350-1356.	3.2	55

#	Article	IF	Citations
820	Determination of geometric and electronic structures of organic crystals from first principles: Role of the molecular configuration on the electronic structure. Journal of Applied Physics, 2017, 121, 045501.	1.1	14
821	Acid Gas Adsorption on Metalâ€“Organic Framework Nanosheets as a Model of an â€œAll-Surfaceâ€• Material. Journal of Chemical Theory and Computation, 2017, 13, 1341-1350.	2.3	23
822	A van der Waals Inclusive Density Functional Theory Study of the Nature of Bonding for Thiophene Adsorption on Ni(100) and Cu(100) Surfaces. Journal of Physical Chemistry C, 2017, 121, 6090-6103.	1.5	19
823	Energy level alignment at molecule-metal interfaces from an optimally tuned range-separated hybrid functional. Journal of Chemical Physics, 2017, 146, .	1.2	59
824	First-Principles Models for van der Waals Interactions in Molecules and Materials: Concepts, Theory, and Applications. Chemical Reviews, 2017, 117, 4714-4758.	23.0	408
825	Semiconductorâ€toâ€Metal Transition and Quasiparticle Renormalization in Doped Graphene Nanoribbons. Advanced Electronic Materials, 2017, 3, 1600490.	2.6	33
826	Surface Interactions and Confinement of Methane: A High Pressure Magic Angle Spinning NMR and Computational Chemistry Study. Langmuir, 2017, 33, 1359-1367.	1.6	22
827	Pathways of NO adsorption on Si(100)2Ã—1 by van der Waals corrected DFT. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750009.	1.8	1
828	Magnetism in a graphene- 4fâ^'3d hybrid system. Physical Review B, 2017, 95, .	1.1	22
829	Rehabilitation of the Perdew-Burke-Ernzerhof generalized gradient approximation for layered materials. Physical Review B, 2017, 95, .	1.1	91
830	Half Layer By Half Layer Growth of a Blue Phosphorene Monolayer on a GaN(001) Substrate. Physical Review Letters, 2017, 118, 046101.	2.9	149
831	Standard grids for highâ€precision integration of modern density functionals: SGâ€2 and SGâ€3. Journal of Computational Chemistry, 2017, 38, 869-882.	1.5	70
832	High-Precision Shock Wave Measurements of Deuterium: Evaluation of Exchange-Correlation Functionals at the Molecular-to-Atomic Transition. Physical Review Letters, 2017, 118, 035501.	2.9	68
833	Competition of van der Waals and chemical forces on goldâ€“sulfur surfaces and nanoparticles. Nature Reviews Chemistry, 2017, 1, .	13.8	95
834	Van Der Waals heterogeneous layerâ€layer carbon nanostructures involving ï€Â·Â·Â·Hâ€Câ€Câ€HÂ·Â·Â·ï€Â·Â·Â·Hâ€Câ€Câ€H stacking based on graphene and graphane sheets. Journal of Computational Chemistry, 2017, 38, 730-739.	1.5	14
835	Towards an accurate description of perovskite ferroelectrics: exchange and correlation effects. Scientific Reports, 2017, 7, 43482.	1.6	57
836	First-principles study of paraelectric and ferroelectric<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="bold">CsH</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">PO</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>including dispersion forces: Stability and related vibrational, dielectric, and elastic properties. Physical Review B, 2017, 95, .	1.1	15
837	Comparing van der Waals DFT methods for water on NaCl(001) and MgO(001). Journal of Chemical Physics, 2017, 146, 064703.	1.2	29

#	Article	IF	Citations
838	The role of water in the elastic properties of aluminosilicate zeolites: DFT investigation. Journal of Molecular Modeling, 2017, 23, 68.	0.8	11
839	Manipulating energy storage characteristics of ultrathin boron carbide monolayer under varied scandium doping. RSC Advances, 2017, 7, 8598-8605.	1.7	30
840	CO₂ Capture and Separations Using MOFs: Computational and Experimental Studies. Chemical Reviews, 2017, 117, 9674-9754.	23.0	837
841	Assessing DFT-D3 Damping Functions Across Widely Used Density Functionals: Can We Do Better?. Journal of Chemical Theory and Computation, 2017, 13, 2043-2052.	2.3	71
842	Influence of Pd/Pd 2 decoration on the structural, electronic and sensing properties of monolayer graphene in the presence of methane molecule: A dispersion-corrected DFT study. Surface Science, 2017, 662, 93-101.	0.8	21
843	The first-principles investigations on magnetic ground-state in Sm-doped phenanthrene. AIP Advances, 2017, 7, 055704.	0.6	3
844	Low-temperature activation of methane on the IrO ₂ (110) surface. Science, 2017, 356, 299-303.	6.0	244
845	Tunable Schottky Barrier at MoSe₂/Metal Interfaces with a Buffer Layer. Journal of Physical Chemistry C, 2017, 121, 9305-9311.	1.5	45
846	Waterâ€“Ice Analogues of Polycyclic Aromatic Hydrocarbons: Water Nanoclusters on Cu(111). Journal of the American Chemical Society, 2017, 139, 6403-6410.	6.6	32
847	Understanding the Fate of Insensitive Munitions Compounds: Computational Study on Adsorption of Nitroguanidine (NQ) and 1,1-Diamino-2,2-dinitroethylene (FOX7) on Pristine and Al-Hydroxylated Î±-Alumina Surfaces. Journal of Physical Chemistry C, 2017, 121, 11560-11567.	1.5	8
848	Oxygen- and Sulfur-Bridged Bianthracene V-Shaped Organic Semiconductors. Bulletin of the Chemical Society of Japan, 2017, 90, 931-938.	2.0	28
849	Tuning the Adsorption of Polysulfides in Lithiumâ€“Sulfur Batteries with Metalâ€“Organic Frameworks. Chemistry of Materials, 2017, 29, 4932-4939.	3.2	98
850	Adsorption of methylene blue and its N-demethylated derivatives on the (111) face of coinage metals: The importance of dispersion interactions. Journal of Chemical Physics, 2017, 146, 164701.	1.2	17
851	Dissecting the role of dispersion on the quantum topology phase diagram of monosaccharide isomers. Monatshefte FÃ¼r Chemie, 2017, 148, 1269-1276.	0.9	7
852	A hybrid organic-inorganic perovskite dataset. Scientific Data, 2017, 4, 170057.	2.4	112
853	Noncovalent Interactions between Dopamine and Regular and Defective Graphene. ChemPhysChem, 2017, 18, 2065-2080.	1.0	27
854	Influence of a graphene surface on the first steps of the hydrogenation of a coronene molecule. Chemical Physics Letters, 2017, 679, 225-232.	1.2	8
855	Adsorption and Formation of Small Na Clusters on Pristine and Double-Vacancy Graphene for Anodes of Na-Ion Batteries. ACS Applied Materials & Interfaces, 2017, 9, 17076-17084.	4.0	42

#	Article	IF	Citations
856	A van der Waals DFT study of chain length dependence of alkanethiol adsorption on Au(111): physisorption vs. chemisorption. Physical Chemistry Chemical Physics, 2017, 19, 13756-13766.	1.3	23
857	Exchange functionals based on finite uniform electron gases. Journal of Chemical Physics, 2017, 146, 114108.	1.2	18
858	Performance of van der Waals Corrected Functionals for Guest Adsorption in the M₂(dobdc) Metalâ€“Organic Frameworks. Journal of Physical Chemistry A, 2017, 121, 4139-4151.	1.1	41
859	Vibrational Excitation of H₂ Scattering from Cu(111): Effects of Surface Temperature and of Allowing Energy Exchange with the Surface. Journal of Physical Chemistry C, 2017, 121, 13617-13633.	1.5	26
860	Hydrogen-Bonding Evolution during the Polymorphic Transformations in CH₃NH₃PbBr₃: Experiment and Theory. Chemistry of Materials, 2017, 29, 5974-5981.	3.2	80
861	Rotational Energy Barriers and Relaxation Times of the Organic Cation in Cubic Methylammonium Lead/Tin Halide Perovskites from First Principles. Journal of Physical Chemistry C, 2017, 121, 14051-14059.	1.5	21
862	Powder diffraction and crystal structure prediction identify four new coumarin polymorphs. Chemical Science, 2017, 8, 4926-4940.	3.7	97
863	Ab initio and classical atomistic modelling of structure and defects inÂcrystalline orthorhombic polyethylene: Twin boundaries, slip interfaces, and nature of barriers. Polymer, 2017, 121, 234-246.	1.8	19
864	van der Waals Contribution to the Relative Stability of Aqueous Zn(2+) Coordination States. Journal of Chemical Theory and Computation, 2017, 13, 3340-3347.	2.3	10
865	Synthesis, characterization and theoretical study in gaseous and solid phases of the imine 4-Acetyl-N-(4-methoxybenzylidene)aniline. Journal of Molecular Structure, 2017, 1147, 300-309.	1.8	2
866	Thirty years of density functional theory in computational chemistry: an overview and extensive assessment of 200 density functionals. Molecular Physics, 2017, 115, 2315-2372.	0.8	1,401
867	The magnetic proximity effect and electrical field tunable valley degeneracy in MoS₂/EuS van der Waals heterojunctions. Nanoscale, 2017, 9, 9502-9509.	2.8	64
868	Phase diagram of waterâ€“methane by first-principles thermodynamics: discovery of MH-IV and MH-V hydrates. Physical Chemistry Chemical Physics, 2017, 19, 15996-16002.	1.3	12
869	Buckyball sandwiches. Science Advances, 2017, 3, e1700176.	4.7	50
870	Ab initio DFT studies of adsorption characteristics of benzene on close-packed surfaces of transition metals. Computational Materials Science, 2017, 137, 10-19.	1.4	9
871	Dispersion-Corrected Spin-Component-Scaled Double-Hybrid Density Functional Theory: Implementation and Performance for Non-covalent Interactions. Journal of Chemical Theory and Computation, 2017, 13, 2650-2666.	2.3	8
872	Using density functional theory to increase the accuracy of experimental crystal structures: The case of potassium peroxocarbonate. Journal of Molecular Structure, 2017, 1146, 1-4.	1.8	1
873	Searching for DFT-based methods that include dispersion interactions to calculate the physisorption of H2 on benzene and graphene. Journal of Chemical Physics, 2017, 146, 214104.	1.2	30

#	Article	IF	Citations
874	libvdwxc: a library for exchangeâ€“correlation functionals in the vdW-DF family. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 065004.	0.8	28
875	Can DFT and ab initio methods adequately describe binding energies in strongly interacting C6X6â‹¯C2X Ï€â€“Ï€ complexes?. Chemical Physics, 2017, 493, 12-19.	0.9	7
876	Double-layer ice from first principles. Physical Review B, 2017, 95, .	1.1	29
877	Deriving phosphorus atomic chains from few-layer black phosphorus. Nano Research, 2017, 10, 2519-2526.	5.8	26
878	Assessment of van der Waals inclusive density functional theory methods for layered electroactive materials. Physical Chemistry Chemical Physics, 2017, 19, 10133-10139.	1.3	43
879	Edge stacking dislocations in two-dimensional bilayers with a small lattice mismatch. Physica E: Low-Dimensional Systems and Nanostructures, 2017, 90, 49-54.	1.3	4
880	Metalâ€“organic and covalent organic frameworks as single-site catalysts. Chemical Society Reviews, 2017, 46, 3134-3184.	18.7	861
881	Description of adenine and cytosine on Au(111) nano surface using different DFT functionals (PW91PW91, wB97XD, M06-2X, M06-L and CAM-B3LYP) in the framework of ONIOM scheme: Non-periodic calculations. Chemical Physics, 2017, 488-489, 1-10.	0.9	36
882	Opinion: Quantum solutions for a sustainable energy future. Nature Reviews Chemistry, 2017, 1, .	13.8	18
883	How strongly do hydrogen and water molecules stick to carbon nanomaterials?. Journal of Chemical Physics, 2017, 146, .	1.2	38
884	Is High-Density Amorphous Ice Simply a â€œDerailedâ€•State along the Ice I to Ice IV Pathway?. Journal of Physical Chemistry Letters, 2017, 8, 1645-1650.	2.1	38
885	Liquid Sulfur Impregnation of Microporous Carbon Accelerated by Nanoscale Interfacial Effects. Nano Letters, 2017, 17, 2517-2523.	4.5	16
886	Trends in the Surface and Catalytic Chemistry of Transition-Metal Ceramics in the Deoxygenation of a Woody Biomass Pyrolysis Model Compound. ACS Catalysis, 2017, 7, 3169-3180.	5.5	32
887	Embedded and DFT Calculations on the Crystal Structures of Small Alkanes, Notably Propane. Crystal Growth and Design, 2017, 17, 1636-1646.	1.4	18
888	Molecule-decorated rutile-type ZnF 2 (110): A periodic DFT study. Surface Science, 2017, 662, 34-41.	0.8	5
889	Interlayer locking and atomic-scale friction in commensurate small-diameter boron nitride nanotubes. Physical Review B, 2017, 95, .	1.1	5
890	Interfacial engineering of phthalocyanine molecules on graphitic and metal substrates. Molecular Simulation, 2017, 43, 384-393.	0.9	2
891	The Solvation Structure of Lithium Ions in an Ether Based Electrolyte Solution from First-Principles Molecular Dynamics. Journal of Physical Chemistry B, 2017, 121, 180-188.	1.2	41

#	Article	IF	Citations
892	Use of the rVV10 Nonlocal Correlation Functional in the B97M-V Density Functional: Defining B97M-rV and Related Functionals. Journal of Physical Chemistry Letters, 2017, 8, 35-40.	2.1	78
893	Î±-Amino Thiophene on Si(100)2 Ã— 1: Adsorption and transition states investigated by van der Waals corrected DFT and CI-NEB. Journal of Theoretical and Computational Chemistry, 2017, 16, 1740001.	1.8	2
894	Firstâ€principles modeling of molecular crystals: structures and stabilities, temperature and pressure. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1294.	6.2	141
895	Density functional theory for modelling large molecular adsorbateâ€“surface interactions: a mini-review and worked example. Molecular Simulation, 2017, 43, 327-345.	0.9	39
896	Exchange-Hole Dipole Dispersion Model for Accurate Energy Ranking in Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2017, 13, 441-450.	2.3	56
897	Weak binding mode of CH 4 on rutile crystallites from density functional theory calculations. Computational and Theoretical Chemistry, 2017, 1121, 11-28.	1.1	3
898	Effect of Molecular Guest Binding on the dâ€“d Transitions of Ni²⁺ of CPO-27-Ni: A Combined UVâ€“Vis, Resonant-Valence-to-Core X-ray Emission Spectroscopy, and Theoretical Study. Inorganic Chemistry, 2017, 56, 14408-14425.	1.9	22
899	Size-Matching Ligand Insertion in MOF-74 for Enhanced CO₂ Capture under Humid Conditions. Journal of Physical Chemistry C, 2017, 121, 24444-24451.	1.5	34
900	Electrochemical Reduction of CO2 on IrxRu(1â€“x)O2(110) Surfaces. ACS Catalysis, 2017, 7, 8502-8513.	5.5	16
901	Improving the Efficiency of Beyond-RPA Methods within the Dielectric Matrix Formulation: Algorithms and Applications to the A24 and S22 Test Sets. Journal of Chemical Theory and Computation, 2017, 13, 5432-5442.	2.3	16
902	Nature of Interlayer Binding and Stacking of spâ€“sp² Hybridized Carbon Layers: A Quantum Monte Carlo Study. Journal of Chemical Theory and Computation, 2017, 13, 5639-5646.	2.3	27
903	N-Heterocyclic carbenes on close-packed coinage metal surfaces: bis-carbene metal adatom bonding scheme of monolayer films on Au, Ag and Cu. Chemical Science, 2017, 8, 8301-8308.	3.7	87
904	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	0.7	4,303
905	Inversion Domain Boundary Induced Stacking and Bandstructure Diversity in Bilayer MoSe₂. Nano Letters, 2017, 17, 6653-6660.	4.5	51
906	First Principle Study on the Adsorption of Hydrocarbon Chains Involved in Fischerâ€“Tropsch Synthesis over Iron Carbides. Journal of Physical Chemistry C, 2017, 121, 25052-25063.	1.5	16
907	Atomistic Simulations of the Crystallization and Aging of GeTe Nanowires. Journal of Physical Chemistry C, 2017, 121, 23827-23838.	1.5	42
908	Modulating the electronic and optical properties of monolayer arsenene phases by organic molecular doping. Nanotechnology, 2017, 28, 495202.	1.3	22
909	Cp-Graphyne: A Low-Energy Graphyne Polymorph with Double Distorted Dirac Points. ACS Omega, 2017, 2, 6822-6830.	1.6	41

#	Article	IF	Citations
910	Structural and electronic changes of pentacene induced by potassium doping. Physical Review B, 2017, 95, .	1.1	4
911	Energetics and electronic structures of thin films and heterostructures of a hexagonal GaN sheet. Japanese Journal of Applied Physics, 2017, 56, 065201.	0.8	5
912	Effect of Surface Structure of TiO₂ Nanoparticles on CO₂ Adsorption and SO₂ Resistance. ACS Sustainable Chemistry and Engineering, 2017, 5, 9295-9306.	3.2	49
913	Benchmark Databases of Intermolecular Interaction Energies: Design, Construction, and Significance. Annual Reports in Computational Chemistry, 2017, 13, 3-91.	0.9	8
914	Image potential states from the van der Waals density functional. Journal of Chemical Physics, 2017, 147, 044708.	1.2	8
915	Stacking in incommensurate graphene/hexagonal-boron-nitride heterostructures based on ab initio study of interlayer interaction. Physical Review B, 2017, 96, .	1.1	23
916	Theoretical Studies on the Growth Mechanism of Chemical Vapor Deposition of Graphene on Metal Surface. , 2017, , 205-241.		0
917	Computational Characterization of the Dependence of Halide Perovskite Effective Masses on Chemical Composition and Structure. Journal of Physical Chemistry C, 2017, 121, 23886-23895.	1.5	38
918	Surface Chemistry Mechanism of Ultra-Low Interfacial Resistance in the Solid-State Electrolyte Li₇La₃Zr₂O₁₂. Chemistry of Materials, 2017, 29, 7961-7968.	3.2	612
919	Low-energy transmission electron diffraction and imaging of large-area graphene. Science Advances, 2017, 3, e1603231.	4.7	35
920	The Positive Role of Hydrogen on the Dehydrogenation of Propane on Pt(111). ACS Catalysis, 2017, 7, 7495-7508.	5.5	95
921	Tuning the topological states in metal-organic bilayers. Physical Review B, 2017, 96, .	1.1	15
922	Computational Study of Low Interlayer Friction in Ti_{n+1}C_n (n = 1, 2, and 3) MXene. ACS Applied Materials & Interfaces, 2017, 9, 34467-34479.	4.0	93
923	CO2 adsorption on the copper surfaces: van der Waals density functional and TPD studies. Journal of Chemical Physics, 2017, 147, 094702.	1.2	47
924	Structural and electronic properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math> -(BEDT-TTF) <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">I</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> , <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi></mml:math>		

#	Article	IF	Citations
928	Multivalency-Driven Formation of Te-Based Monolayer Materials: A Combined First-Principles and Experimental study. Physical Review Letters, 2017, 119, 106101.	2.9	409
929	Adsorption of graphene to metal (111) surfaces using the exchange-hole dipole moment model. Carbon, 2017, 124, 531-540.	5.4	22
930	Ultrahigh mobility and efficient charge injection in monolayer organic thin-film transistors on boron nitride. Science Advances, 2017, 3, e1701186.	4.7	146
931	Synergy of van der Waals and self-interaction corrections in transition metal monoxides. Physical Review B, 2017, 96, .	1.1	50
932	Interaction of CO with an hBN surface doped with Ti and Pt: A First Principles Study. Journal of Physics: Conference Series, 2017, 792, 012074.	0.3	1
933	Structure of graphite-like BC 2 layer in Sc 2 B 1.1 C 3.2 : An intermediate between BC and BC 3. Journal of Solid State Chemistry, 2017, 254, 144-149.	1.4	3
934	Molecular Picture of the Adsorption of Ibuprofen and Benzoic Acid on Hydrated Amorphous Silica through DFT-D Calculations Combined with Solid-State NMR Experiments. Journal of Physical Chemistry C, 2017, 121, 17339-17347.	1.5	22
935	Nonlinear atomic vibrations and structural phase transitions in strained carbon chains. Computational Materials Science, 2017, 138, 353-367.	1.4	16
936	Evidence for Ultralow-Energy Vibrations in Large Organic Molecules. Nano Letters, 2017, 17, 4929-4933.	4.5	11
937	The interaction of proteins with silica surfaces. Part I: Ab initio modeling. Computational and Theoretical Chemistry, 2017, 1117, 100-107.	1.1	6
938	Periodic density functional theory analysis of direct methane conversion into ethylene and aromatic hydrocarbons catalyzed by Mo₄C₂/ZSM-5. Physical Chemistry Chemical Physics, 2017, 19, 22243-22255.	1.3	14
939	Assessment of two hybrid van der Waals density functionals for covalent and non-covalent binding of molecules. Journal of Chemical Physics, 2017, 146, 234106.	1.2	33
940	Simulation and understanding of atomic and molecular quantum crystals. Reviews of Modern Physics, 2017, 89, .	16.4	94
941	The role of van der Waals and exchange interactions in high-pressure solid hydrogen. Physical Chemistry Chemical Physics, 2017, 19, 21829-21839.	1.3	23
942	Simple way to apply nonlocal van der Waals functionals within all-electron methods. Physical Review B, 2017, 96, .	1.1	16
943	Creating anisotropic spin-split surface states in momentum space by molecular adsorption. Physical Review B, 2017, 96, .	1.1	6
944	High performance material for hydrogen storage: Graphenelike Si2BN solid. International Journal of Hydrogen Energy, 2017, 42, 22942-22952.	3.8	50
945	Modelling pH and potential in dynamic structures of the water/Pt(111) interface on the atomic scale. Physical Chemistry Chemical Physics, 2017, 19, 23505-23514.	1.3	48

#	Article	IF	Citations
946	An organic-inorganic perovskite ferroelectric with large piezoelectric response. Science, 2017, 357, 306-309.	6.0	744
947	Experimental and ab initio molecular dynamics study of the structure and physical properties of liquid GeTe. Physical Review B, 2017, 96, .	1.1	33
948	Formaldehyde adsorption on graphane. Computational and Theoretical Chemistry, 2017, 1117, 119-123.	1.1	14
949	SBH10: A Benchmark Database of Barrier Heights on Transition Metal Surfaces. Journal of Physical Chemistry C, 2017, 121, 19807-19815.	1.5	89
950	Annealing of ion-irradiated hexagonal boron nitride on Ir(111). Physical Review B, 2017, 96, .	1.1	17
951	Mitigating Cation Diffusion Limitations and Intercalation-Induced Framework Transitions in a 1D Tunnel-Structured Polymorph of V₂O₅. Chemistry of Materials, 2017, 29, 10386-10397.	3.2	24
952	Insights on the Role of Many-Body Polarization Effects in the Wetting of Graphitic Surfaces by Water. Journal of Physical Chemistry C, 2017, 121, 28166-28179.	1.5	46
953	Highly Tunable Electronic Structures of Phosphorene/Carbon Nanotube Heterostructures through External Electric Field and Atomic Intercalation. Nano Letters, 2017, 17, 7995-8004.	4.5	15
954	Properties of Highly Oriented Pyrolytic Graphite Supported TaSi₁₆ Clusters: A Density Functional Investigation. Journal of Physical Chemistry C, 2017, 121, 28490-28497.	1.5	9
955	MoirÃ©-pattern interlayer potentials in van der Waals materials in the random-phase approximation. Physical Review B, 2017, 96, .	1.1	19
956	Trends in Adhesion Energies of Gold on MgO(100), Rutile TiO₂(110), and CeO₂(111) Surfaces: A Comparative DFT Study. Journal of Physical Chemistry C, 2017, 121, 28328-28338.	1.5	29
957	Theoretical Study on Rotational Controllability of Organic Cations in Organicâ€“Inorganic Hybrid Perovskites: Hydrogen Bonds and Halogen Substitution. Journal of Physical Chemistry C, 2017, 121, 26188-26195.	1.5	19
958	Unveiling orbital coupling at the CoPc/Bi(111) surface by ab initio calculations and photoemission spectroscopy. RSC Advances, 2017, 7, 52143-52150.	1.7	1
959	Mechanism of enhancement of ferroelectricity of croconic acid with temperature. Physical Chemistry Chemical Physics, 2017, 19, 32216-32225.	1.3	7
960	Confinement and fermion doubling problem in Dirac-like Hamiltonians. Physical Review B, 2017, 96, .	1.1	16
961	Evaluation of Multivalent Cation Insertion in Single- and Double-Layered Polymorphs of V₂O₅. ACS Applied Materials & Interfaces, 2017, 9, 23756-23765.	4.0	64
962	Anomalous in-plane anisotropic Raman response of monoclinic semimetal 1â€‰TÂ´-MoTe 2. Scientific Reports, 2017, 7, 1758.	1.6	47
963	A DFT study of H-dissolution into the bulk of a crystalline Ni(111) surface: a chemical identifier for the reaction kinetics. Physical Chemistry Chemical Physics, 2017, 19, 19150-19158.	1.3	29

#	Article	IF	Citations
964	Origins of the structural phase transitions in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoTe</mml:mi><mml:mn>2</mml:mn></mml:msub></m and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>WTe</mml:mi><mml:mn>2</mml:mn></mml:msub></mn Physical Review B, 2017, 95, .	1.1	97
965	Ground state structure of high-energy-density polymeric carbon monoxide. Physical Review B, 2017, 95, .	1.1	22
966	Electronic Structure of Edge-Modified Graphene Quantum Dots Interacting with Polyaniline: Vibrational and Optical Properties. Journal of Physical Chemistry C, 2017, 121, 16576-16583.	1.5	21
967	Halo-substituted azobenzenes adsorbed at Ag(111) and Au(111) interfaces: Structures and optical properties. Physical Review B, 2017, 95, .	1.1	2
968	Efficient mixed-solvent exfoliation of few-quintuple layer Bi₂S₃and its photoelectric response. Nanotechnology, 2017, 28, 335602.	1.3	23
969	Origin of the Strong Interaction between Polar Molecules and Copper(II) Paddle-Wheels in Metal Organic Frameworks. Journal of Physical Chemistry C, 2017, 121, 15135-15144.	1.5	23
970	Computational design of a robust two-dimensional antiferromagnetic semiconductor. Physical Review B, 2017, 96, .	1.1	20
971	Finite-temperature properties of nonmagnetic transition metals: Comparison of the performance of constraint-based semilocal and nonlocal functionals. Physical Review B, 2017, 95, .	1.1	35
972	Ionic and superionic phases in ammonia dihydrate <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">N</mml:mi><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mo>Â·</mml:mo><mml:mn>2</mml:mn><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:math> under high pressure. Physical Review B,	1.1	21
973	Graphenylene Monolayers Doped with Alkali or Alkaline Earth Metals: Promising Materials for Clean Energy Storage. Journal of Physical Chemistry C, 2017, 121, 14393-14400.	1.5	65
974	Methylbenzenes on graphene. Surface Science, 2017, 664, 162-167.	0.8	15
975	Terahertz Absorption by Cellulose: Application to Ancient Paper Artifacts. Physical Review Applied, 2017, 7, .	1.5	32
976	CO-induced Pd segregation and the effect of subsurface Pd on CO adsorption on CuPd surfaces. Journal of Physics Condensed Matter, 2017, 29, 025005.	0.7	11
977	Reduced work function of graphene by metal adatoms. Applied Surface Science, 2017, 394, 98-107.	3.1	36
978	Recent developments of firstâ€principles force fields. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1282.	6.2	18
979	Comparison of performance of van der Waals-corrected exchange-correlation functionals for interlayer interaction in graphene and hexagonal boron nitride. Computational Materials Science, 2017, 128, 45-58.	1.4	72
980	Highâ€Electronâ€Mobility and Airâ€Stable 2D Layered PtSe₂ FETs. Advanced Materials, 2017, 29, 1604230.	11.1	502
981	Ab initio study of stability and migration of point defects in copper-graphene layered composite. Journal of Alloys and Compounds, 2017, 692, 49-58.	2.8	22

#	Article	IF	Citations
982	Phase Equilibria and Condensed Phase Properties of Fluorinated Alkanes via First Principles Simulations. ChemistrySelect, 2017, 2, 11969-11976.	0.7	4
983	Structural and antiferromagnetic properties of Sm-doped chrysene. AIP Advances, 2017, 7, 055707.	0.6	2
984	Strain-induced charge transfer and polarity control of a heterosheet comprising C₆₀and graphene. Applied Physics Express, 2017, 10, 095101.	1.1	6
985	Sterically controlled mechanochemistry under hydrostatic pressure. Nature, 2018, 554, 505-510.	13.7	71
986	Ab-initio study of structural and electronic properties of WS2/h-BN van der Waals heterostructure. Surface Science, 2018, 672-673, 13-18.	0.8	11
987	Deciphering Anomalous Raman Features of Regioregular Poly(3-hexylthiophene) in Ordered Aggregation Form. Journal of Physical Chemistry C, 2018, 122, 4224-4231.	1.5	18
988	Computational Screening of Hydration Reactions for Thermal Energy Storage: New Materials and Design Rules. Chemistry of Materials, 2018, 30, 2006-2017.	3.2	45
989	Diffusion of Sticky Nanoparticles in a Polymer Melt: Crossover from Suppressed to Enhanced Transport. Macromolecules, 2018, 51, 2268-2275.	2.2	52
990	GAtor: A First-Principles Genetic Algorithm for Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2018, 14, 2246-2264.	2.3	86
991	Clathrate ice sL: a new crystalline phase of ice with ultralow density predicted by first-principles phase diagram computations. Physical Chemistry Chemical Physics, 2018, 20, 8333-8340.	1.3	23
992	Insights into the Structure of Liquid Water from Nuclear Quantum Effects on the Density and Compressibility of Ice Polymorphs. Journal of Physical Chemistry B, 2018, 122, 5694-5706.	1.2	11
993	Composite and Low-Cost Approaches for Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2018, 14, 2265-2276.	2.3	18
994	First-principles investigation of surface properties and adsorption of oxygen on Ni-22Cr and the role of molybdenum. Corrosion Science, 2018, 134, 103-111.	3.0	37
995	Structural and electronic properties of the V-V compounds isoelectronic to GaN and isostructural to gray arsenic. Materials Research Express, 2018, 5, 035904.	0.8	2
996	Imaging Catalytic Activation of CO₂ on Cu₂O (110): A First-Principles Study. Chemistry of Materials, 2018, 30, 1912-1923.	3.2	56
997	Transferability of CO₂ Force Fields for Prediction of Adsorption Properties in All-Silica Zeolites. Journal of Physical Chemistry C, 2018, 122, 10892-10903.	1.5	12
998	An experimental and computational study of CO2adsorption in the sodalite-type M-BTT (M = Cr, Mn, Fe,) Tj ETQq0 0 0 rgBT /Overlock 10	3.7	43
999	Density Functional Theory Modeling of Solid-State Nuclear Magnetic Resonances for Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry C, 2018, 122, 11008-11014.	1.5	0

#	Article	IF	Citations
1000	Strain-Tuning Atomic Substitution in Two-Dimensional Atomic Crystals. ACS Nano, 2018, 12, 4853-4860.	7.3	75
1001	Structural and electronic properties of V₂O₅ and their tuning by doping with 3d elements â€“ modelling using the DFT+U method and dispersion correction. Physical Chemistry Chemical Physics, 2018, 20, 13934-13943.	1.3	41
1002	Atomic Orbital Implementation of Extended Symmetry-Adapted Perturbation Theory (XSAPT) and Benchmark Calculations for Large Supramolecular Complexes. Journal of Chemical Theory and Computation, 2018, 14, 2955-2978.	2.3	43
1003	Atomistic Elucidation of Sorption Processes in Hydrogen Evolution Reaction on a van der Waals Heterostructure. Journal of Physical Chemistry C, 2018, 122, 10034-10041.	1.5	18
1004	Equilibration and analysis of first-principles molecular dynamics simulations of water. Journal of Chemical Physics, 2018, 148, 124501.	1.2	41
1005	Origin of the monolayer Raman signature in hexagonal boron nitride: a first-principles analysis. Journal of Physics Condensed Matter, 2018, 30, 185701.	0.7	3
1006	Strain tuning of electronic properties of various dimension elemental tellurium with broken screw symmetry. Journal of Physics Condensed Matter, 2018, 30, 125001.	0.7	26
1007	Theoretical investigations of the anisotropic optical properties of distorted <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mspace width="0.16em" /><mml:msub><mml:mi>ReS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ReSe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml	1.1	53
1008	Signatures of van der Waals binding: A coupling-constant scaling analysis. Physical Review B, 2018, 97, .	1.1	17
1009	DFT study of stabilization effects on N-doped graphene for ORR catalysis. Catalysis Today, 2018, 312, 118-125.	2.2	81
1010	Benchmarking several van der Waals dispersion approaches for the description of intermolecular interactions. Journal of Chemical Physics, 2018, 148, 064112.	1.2	37
1011	Structural and Bonding Characteristics of Potassium-Doped p-Terphenyl Superconductors. Journal of Physical Chemistry C, 2018, 122, 3801-3808.	1.5	36
1012	Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds. Nature Nanotechnology, 2018, 13, 246-252.	15.6	1,317
1013	Density functional theory study of inter-layer coupling in bulk tin selenide. Chemical Physics Letters, 2018, 695, 200-204.	1.2	24
1014	Atomic Structure of Intrinsic and Electron-Irradiation-Induced Defects in MoTe₂. Chemistry of Materials, 2018, 30, 1230-1238.	3.2	56
1015	Water adsorbate phases on ZnO and impact of vapor pressure on the equilibrium shape of nanoparticles. Journal of Chemical Physics, 2018, 148, 054701.	1.2	11
1016	Electronic Exchange and Correlation in van der Waals Systems: Balancing Semilocal and Nonlocal Energy Contributions. Journal of Chemical Theory and Computation, 2018, 14, 1361-1369.	2.3	25
1017	An Aqueous Inorganic Polymer Binder for High Performance Lithiumâ€“Sulfur Batteries with Flame-Retardant Properties. ACS Central Science, 2018, 4, 260-267.	5.3	147

#	Article	IF	Citations
1018	Investigation of the Ligandâ€“Nanoparticle Interface: A Cryogenic Approach for Preserving Surface Chemistry. Journal of Physical Chemistry C, 2018, 122, 3582-3590.	1.5	12
1019	Benchmark Database of Transition Metal Surface and Adsorption Energies from Many-Body Perturbation Theory. Journal of Physical Chemistry C, 2018, 122, 4381-4390.	1.5	53
1020	Chemical modification of group IV graphene analogs. Science and Technology of Advanced Materials, 2018, 19, 76-100.	2.8	33
1021	Realization of a half-metallic state on bilayer WSe₂ using doping transition metals (Cr,) Tj ETQq1 1 0.784314 rgBT /Over	1.3	20
1022	Crystal Structures and Electronic Properties of Xeâ€“Cl Compounds at High Pressure. Journal of Physical Chemistry C, 2018, 122, 2941-2950.	1.5	7
1023	Density Functional Theory-Based Adsorption Isotherms for Pure and Flue Gas Mixtures on Mg-MOF-74. Application in CO₂ Capture Swing Adsorption Processes. Journal of Physical Chemistry C, 2018, 122, 3945-3957.	1.5	38
1024	X-ray electron density investigation of chemical bonding in van der Waals materials. Nature Materials, 2018, 17, 249-252.	13.3	93
1025	Tunable magnetotransport in Fe/hBN/graphene/hBN/Pt(Fe) epitaxial multilayers. Journal Physics D: Applied Physics, 2018, 51, 095302.	1.3	8
1026	Development of Embedded and Performance of Density Functional Methods for Molecular Crystals. Journal of Physical Chemistry A, 2018, 122, 708-713.	1.1	22
1027	Atomic adsorption on pristine graphene along the Periodic Table of Elements â€“ From PBE to non-local functionals. Applied Surface Science, 2018, 436, 433-440.	3.1	61
1028	First-Principles Study of the Interactions between Graphene Oxide and Amine-Functionalized Carbon Nanotube. Journal of Physical Chemistry C, 2018, 122, 1288-1298.	1.5	17
1029	Equation of state and optical properties of warm dense helium. Physics of Plasmas, 2018, 25, .	0.7	18
1030	Phase Diagram of Hydrogen and a Hydrogen-Helium Mixture at Planetary Conditions by Quantum MonteÂCarlo Simulations. Physical Review Letters, 2018, 120, 025701.	2.9	69
1031	Tuning dispersion correction in DFT-D2 for metal-molecule interactions: A tailored reparameterization strategy for the adsorption of aromatic systems on Ag(1â€¯1â€¯1). Chemical Physics Letters, 2018, 693, 28-33.	1.2	13
1032	Roles of sliding-induced defects and dissociated water molecules on low friction of graphene. Scientific Reports, 2018, 8, 121.	1.6	26
1033	Few-layer Tellurium: one-dimensional-like layered elementary semiconductor with striking physical properties. Science Bulletin, 2018, 63, 159-168.	4.3	207
1034	How do London Dispersion Interactions Impact the Photochemical Processes of Molecular Switches?. Journal of Physical Chemistry Letters, 2018, 9, 464-470.	2.1	22
1035	Comparison of the Performance of van der Waals Dispersion Functionals in the Description of Water and Ethanol on Transition Metal Surfaces. Journal of Physical Chemistry C, 2018, 122, 1577-1588.	1.5	36

#	Article	IF	Citations
1036	Improved Photoactivity of Pyroxene Silicates by Cation Substitutions. ChemPhysChem, 2018, 19, 943-953.	1.0	2
1037	Formic acid decomposition on Pt1/Cu (111) single platinum atom catalyst: Insights from DFT calculations and energetic span model analysis. Applied Surface Science, 2018, 436, 631-638.	3.1	30
1038	Anchoring of Iron Oxyhydroxide Clusters at H and L Ferritin Subunits. ACS Biomaterials Science and Engineering, 2018, 4, 483-490.	2.6	5
1039	Reaction Pathways for Solvent Decomposition on Magnesium Anodes. Journal of Physical Chemistry C, 2018, 122, 10714-10724.	1.5	28
1040	Structural and electronic properties of SnS 2 stacked nanosheets: An ab-initio study. Journal of Physics and Chemistry of Solids, 2018, 120, 211-217.	1.9	11
1041	Controlling the charge transfer flow at the graphene/pyreneâ€“nitrilotriacetic acid interface. Journal of Materials Chemistry C, 2018, 6, 5046-5054.	2.7	18
1042	One Oxygen Vacancy, Two Charge States: Characterization of Reduced Î±-MoO₃(010) through Theoretical Methods. Journal of Physical Chemistry Letters, 2018, 9, 2568-2573.	2.1	43
1043	Benchmarking the Effective Fragment Potential Dispersion Correction on the S22 Test Set. Journal of Physical Chemistry A, 2018, 122, 4076-4084.	1.1	3
1044	Combined Computational and Experimental Study of the Pressure Dependence of the Structural and Vibrational Properties on Solid Naphthalene C₁₀H₈. Materials Science Forum, 2018, 914, 175-181.	0.3	1
1045	Structure, Elastic Constants and XRD Spectra of Extended Solids under High Pressure. MRS Advances, 2018, 3, 499-504.	0.5	2
1046	First-principles study of pollutant molecules absorbed on polymeric adsorbents using the vdW-DF2 functional. Materials Research Express, 2018, 5, 035516.	0.8	4
1047	Comment on â€œTheoretical study of the dynamics of atomic hydrogen adsorbed on graphene multilayersâ€. Physical Review B, 2018, 97, .	1.1	8
1048	Indium selenide monolayer: a two-dimensional material with strong second harmonic generation. CrystEngComm, 2018, 20, 2573-2582.	1.3	16
1049	A Comparative Ab Initio Study of Anhydrous Dehydrogenation of Linear-Chain Alcohols on Cu(110). Journal of Physical Chemistry C, 2018, 122, 7806-7815.	1.5	18
1050	Lowest-Energy Crystalline Polymorphs of P3HT. Journal of Physical Chemistry C, 2018, 122, 9141-9151.	1.5	18
1051	Molecular Modelling of the H₂â€Adsorptive Properties of Tetrazolateâ€Based Metalâ€“Organic Frameworks: From the Cluster Approach to Periodic Simulations. ChemPhysChem, 2018, 19, 1349-1357.	1.0	6
1052	Tuning the optoelectronic characteristics of ionic organic crystalline assemblies. Journal of Materials Chemistry C, 2018, 6, 4041-4056.	2.7	15
1053	Different Molecular Arrangement of Perylene in Metallic and Semiconducting Carbon Nanotubes: Impact of van der Waals Interaction. Journal of Physical Chemistry C, 2018, 122, 5805-5812.	1.5	15

#	Article	IF	Citations
1054	AbÂInitio Calculation of the Miscibility Diagram for Hydrogen-Helium Mixtures. Physical Review Letters, 2018, 120, 115703.	2.9	70
1055	Prediction of a Large-Gap and Switchable Kane-Mele Quantum Spin Hall Insulator. Physical Review Letters, 2018, 120, 117701.	2.9	79
1056	Electronic, Magnetic and Optical Properties of 2D Metal Nanolayers: A DFT Study. Metals and Materials International, 2018, 24, 904-912.	1.8	6
1057	First-principles investigation of the Lewis acidâ€“base adduct formation at the methylammonium lead iodide surface. Physical Chemistry Chemical Physics, 2018, 20, 11183-11195.	1.3	9
1058	Ab Initio Molecular Dynamics and Lattice Dynamics-Based Force Field for Modeling Hexagonal Boron Nitride in Mechanical and Interfacial Applications. Journal of Physical Chemistry Letters, 2018, 9, 1584-1591.	2.1	55
1059	On the hydrogen evolution reaction activity of grapheneâ€“hBN van der Waals heterostructures. Physical Chemistry Chemical Physics, 2018, 20, 15007-15014.	1.3	41
1060	Hydrogen adsorption on decorated graphyne and its analogous with Na. Materials Research Bulletin, 2018, 98, 200-205.	2.7	14
1061	Advances in Molecular Simulation Studies of Clay Minerals. Green Energy and Technology, 2018, , 175-183.	0.4	2
1062	Revitalized interest in vanadium pentoxide as cathode material for lithium-ion batteries and beyond. Energy Storage Materials, 2018, 11, 205-259.	9.5	221
1063	Structural and Electronic Properties of Defectâ€Free and Defectâ€Containing Polypropylene: A Computational Study by van der Waals Densityâ€Functional Method. Physica Status Solidi (B): Basic Research, 2018, 255, 1700036.	0.7	4
1064	The structure of metal-water interface at the potential of zero charge from density functional theory-based molecular dynamics. Journal of Electroanalytical Chemistry, 2018, 819, 87-94.	1.9	50
1065	C3B monolayer as an anchoring material for lithium-sulfur batteries. Carbon, 2018, 129, 38-44.	5.4	105
1066	Highâ€Pressureâ€Induced Comminution and Recrystallization of CH₃NH₃PbBr₃ Nanocrystals as Large Thin Nanoplates. Advanced Materials, 2018, 30, 1705017.	11.1	89
1067	Crystallographic, vibrational modes and optical properties data of Î±-DIPAB crystal. Data in Brief, 2018, 16, 667-684.	0.5	14
1068	Hydrogen-Assisted Epitaxial Growth of Monolayer Tungsten Disulfide and Seamless Grain Stitching. Chemistry of Materials, 2018, 30, 403-411.	3.2	60
1069	First-Principles Calculations of van der Waals and Spin Orbit Effects on the Two-Dimensional Topological Insulator Stanene and Stanene on Ge(111) Substrate. Journal of Superconductivity and Novel Magnetism, 2018, 31, 2579-2588.	0.8	10
1070	Diffusion Kinetics of Gold and Copper Atoms on Pristine and Reduced Rutile TiO₂ (110) Surfaces. Journal of Physical Chemistry C, 2018, 122, 3824-3837.	1.5	12
1071	Atomic adsorption on graphene with a single vacancy: systematic DFT study through the periodic table of elements. Physical Chemistry Chemical Physics, 2018, 20, 858-865.	1.3	81

#	Article	IF	Citations
1072	Joint Experimental and Computational Investigation of the Flexibility of a Diacetyleneâ€Based Mixedâ€Linker MOF: Revealing the Existence of Two Lowâ€Temperature Phase Transitions and the Presence of Colossal Positive and Giant Negative Thermal Expansions. Chemistry - A European Journal, 2018, 24, 1586-1605.	1.7	10
1073	Intermolecular orbital interaction in Ï€ systems. Molecular Physics, 2018, 116, 978-986.	0.8	1
1074	Performance of density functionals for modeling vapor liquid equilibria of CO₂ and SO₂. Journal of Computational Chemistry, 2018, 39, 397-406.	1.5	12
1075	Assessment of DFT for endohedral complexes' dipole moment: PNO-LCCSD-F12 as a reference method. Physical Chemistry Chemical Physics, 2018, 20, 29374-29388.	1.3	3
1076	van der Waals interaction-induced photoluminescence weakening and multilayer growth in epitaxially aligned WS₂. Physical Chemistry Chemical Physics, 2018, 20, 29790-29797.	1.3	7
1077	Charge-governed phase manipulation of few-layer tellurium. Nanoscale, 2018, 10, 22263-22269.	2.8	28
1078	Structures of liquid selenium at high pressures. Journal of Physics: Conference Series, 2018, 946, 012101.	0.3	2
1079	Effect of dispersion corrections on ab initio predictions of graphite and diamond properties under pressure. Physical Review B, 2018, 98, .	1.1	24
1080	Ab Initio Evaluation of Henry Coefficients Using Importance Sampling. Journal of Chemical Theory and Computation, 2018, 14, 6359-6369.	2.3	12
1081	Adsorption and diffusion of sulfur on the (111), (100), (110), and (211) surfaces of FCC metals: Density functional theory calculations. Journal of Chemical Physics, 2018, 149, 204701.	1.2	25
1082	Tuning the balance between dispersion and entropy to design temperature-responsive flexible metal-organic frameworks. Nature Communications, 2018, 9, 4899.	5.8	90
1083	Edge-Functionalized Graphene Nanoribbon Chemical Sensor: Comparison with Carbon Nanotube and Graphene. ACS Applied Materials & Interfaces, 2018, 10, 42905-42914.	4.0	41
1084	Optical Properties of Silicene and Related Materials from First Principles. Nanoscience and Technology, 2018, , 73-98.	1.5	6
1085	Are dispersion corrections accurate outside equilibrium? A case study on benzene. Beilstein Journal of Organic Chemistry, 2018, 14, 1181-1191.	1.3	15
1086	Sensitivity to Dispersion Forces in First-Principles Modeling of Disordered Chalcogenides. Frontiers in Materials, 2018, 5, .	1.2	7
1087	Impact of Lowâ€Frequency Vibrations on Charge Transport in Highâ€Mobility Organic Semiconductors. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1800485.	1.2	11
1088	Firstâ€Principles Study of Aziridinium Lead Iodide Perovskite for Photovoltaics. ChemPhysChem, 2019, 20, 602-607.	1.0	8
1089	Effect of Crystallinity on Li Adsorption in Polyethylene Oxide. Chemistry of Materials, 2018, 30, 8804-8810.	3.2	25

#	Article	IF	Citations
1090	Inelastic Scattering of N2 off W(001): Reconciling Experiment and Theory at Low Collision Energies. Journal of Physical Chemistry C, 2018, 122, 28856-28861.	1.5	6
1091	Elucidating CO₂ Chemisorption in Diamine-Appended Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2018, 140, 18016-18031.	6.6	107
1092	Competing adsorption mechanisms of pyridine on Cu, Ag, Au, and Pt(110) surfaces. Journal of Chemical Physics, 2018, 149, 214703.	1.2	9
1093	Evaluation of exchange-correlation functionals with multiple-shock conductivity measurements in hydrogen and deuterium at the molecular-to-atomic transition. Physical Review B, 2018, 98, .	1.1	17
1094	Dissociation of CHD3 on Cu(111), Cu(211), and single atom alloys of Cu(111). Journal of Chemical Physics, 2018, 149, 224701.	1.2	17
1095	High magnetoresistance in ultra-thin two-dimensional Cr-based MXenes. Nanoscale, 2018, 10, 19492-19497.	2.8	26
1096	Kinetic pathways towards mass production of single crystalline stanene on topological insulator substrates. Nanoscale, 2018, 10, 18988-18994.	2.8	8
1097	Surface-Mediated Aligned Growth of Monolayer MoS₂ and In-Plane Heterostructures with Graphene on Sapphire. ACS Nano, 2018, 12, 10032-10044.	7.3	64
1098	Large magneto-optical effects and magnetic anisotropy energy in two-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">Cr</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mrow><mml:mi mathvariant="normal">Ge</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mrow><mml:mi mathvariant="normal">Te</mml:mi></mml:mrow><mml:mn>6</mml:mn></mml:msub></mml:math>. Physical Review B, 2018, 98, .	1.1	119
1099	Density functional theory study of decalin dehydrogenation for hydrogen release on Pt(111) and Pt(211). International Journal of Hydrogen Energy, 2018, 43, 19575-19588.	3.8	19
1100	A Complex Zeolite Containing Multiple Ring Sizes in a Single Channel: Oneâ€Dimensional Zeolite UZMâ€55. Chemistry - A European Journal, 2018, 24, 17779-17787.	1.7	7
1101	Quantifying Confidence in DFT-Predicted Surface Pourbaix Diagrams of Transition-Metal Electrodeâ€“Electrolyte Interfaces. Langmuir, 2018, 34, 12259-12269.	1.6	57
1102	Ab initio study of the structure, isotope effects, and vibrational properties in KDP crystals. Physical Review B, 2018, 98, .	1.1	19
1103	Ferroelectric polymers exhibiting behaviour reminiscent of a morphotropic phase boundary. Nature, 2018, 562, 96-100.	13.7	200
1104	DFT Study of the Oxygen Reduction Reaction on Carbon-Coated Iron and Iron Carbide. ACS Catalysis, 2018, 8, 10521-10529.	5.5	46
1105	Energy Trends in Adsorption at Surfaces. , 2018, , 1-20.		0
1106	Assessing the Predictive Power of Density Functional Theory in Finite-Temperature Hydrogen Adsorption/Desorption Thermodynamics. Journal of Physical Chemistry C, 2018, 122, 26189-26195.	1.5	5
1107	The Nonlocal Kernel in van der Waals Density Functionals as an Additive Correction: An Extensive Analysis with Special Emphasis on the B97M-V and ï‰B97M-V Approaches. Journal of Chemical Theory and Computation, 2018, 14, 5725-5738.	2.3	170

#	Article	IF	Citations
1108	Selective Reduction of Oxygen Functional Groups to Improve the Response Characteristics of Graphene Oxide-Based Formaldehyde Sensor Device: A First Principle Study. IEEE Transactions on Electron Devices, 2018, , 1-8.	1.6	8
1109	Wafer-Scale Fabrication of Two-Dimensional PtS₂/PtSe₂ Heterojunctions for Efficient and Broad band Photodetection. ACS Applied Materials & Interfaces, 2018, 10, 40614-40622.	4.0	110
1110	Temperature Dependence of Carbon Monoxide Adsorption on a High-Silica H-FER Zeolite. Journal of Physical Chemistry C, 2018, 122, 26088-26095.	1.5	13
1111	Non-Covalent Interactions in Molecular Crystals: Exploring the Accuracy of the Exchange-Hole Dipole Moment Model with Local Orbitals. Journal of Chemical Theory and Computation, 2018, 14, 5715-5724.	2.3	9
1112	Water desorption from rapidly-heated metal oxide surfacesâ€"first principles, molecular dynamics, and the Temkin isotherm. Journal of Physics Condensed Matter, 2018, 30, 465002.	0.7	16
1113	Faraday cage screening reveals intrinsic aspects of the van der Waals attraction. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E10295-E10302.	3.3	12
1114	Stability of Hydrogen Hydrates from Second-Order MÃ¸llerâ€"Plesset Perturbation Theory. Journal of Physical Chemistry Letters, 2018, 9, 5624-5629.	2.1	7
1115	Dispersion-Corrected DFT Struggles with Predicting Three-Body Interaction Energies. Journal of Chemical Theory and Computation, 2018, 14, 5079-5089.	2.3	19
1116	Superconductivity and phase stability of potassium-doped biphenyl. Physical Chemistry Chemical Physics, 2018, 20, 25217-25223.	1.3	31
1117	A first-principles study on the chemical stability of inorganic perovskite solid solutions Cs_{1â^'x}Rb_xPbI₃at finite temperature and pressure. Journal of Materials Chemistry A, 2018, 6, 17994-18002.	5.2	47
1118	Structure and Raman scattering of chained carbon films on copper substrate: ab initio approach. IOP Conference Series: Materials Science and Engineering, 2018, 292, 012102.	0.3	2
1119	First-principles study on the material properties of the inorganic perovskite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Rb</mml:mi><mml:mrow><mml:mn>1</mml:mn> for solar cell applications. Physical Review B, 2018, 98, .	3.7	61
1120	The crucial role of density functional nonlocality and on-axis CH3NH3 rotation induced I2 formation in hybrid organic-inorganic CH3NH3PbI3 cubic perovskite. Scientific Reports, 2018, 8, 13161.	1.6	12
1121	Temperature-programmed desorption studies of NH3 and H2O on the RuO2(110) surface: effects of adsorbate diffusion. Physical Chemistry Chemical Physics, 2018, 20, 24201-24209.	1.3	14
1122	High energetic polymeric nitrogen sheet confined in a graphene matrix. RSC Advances, 2018, 8, 30912-30918.	1.7	14
1123	Predicting the thermodynamic stability of double-perovskite halides from density functional theory. APL Materials, 2018, 6, .	2.2	42
1124	Identifying Few-Molecule Water Clusters with High Precision on Au(111) Surface. ACS Nano, 2018, 12, 6452-6457.	7.3	25
1125	First principle study of chain termination reactions during Fischer-Tropsch Synthesis on Ï‡ -Fe 5 C 2 (010). Molecular Catalysis, 2018, 453, 55-63.	1.0	8

#	Article	IF	Citations
1126	Zinc oxideâ€“black phosphorus composites for ultrasensitive nitrogen dioxide sensing. Nanoscale Horizons, 2018, 3, 525-531.	4.1	52
1127	Enhancement of CO₂ binding and mechanical properties upon diamine functionalization of M₂(dobpdc) metalâ€“organic frameworks. Chemical Science, 2018, 9, 5197-5206.	3.7	39
1128	Quantum Monte Carlo calculations of van der Waals interactions between aromatic benzene rings. Physical Review B, 2018, 97, .	1.1	6
1129	Extent of Fock-exchange mixing for a hybrid van der Waals density functional?. Journal of Chemical Physics, 2018, 148, 194115.	1.2	17
1130	Investigating the adsorption of nitrobenzene on M/Pd (1â€¯1â€¯1) bimetallic surface as an effective catalyst. Applied Surface Science, 2018, 454, 343-349.	3.1	9
1131	Elemental Identification by Combining Atomic Force Microscopy and Kelvin Probe Force Microscopy. ACS Nano, 2018, 12, 5274-5283.	7.3	37
1132	Effect of adsorbates on single-molecule junction conductance. Surface Science, 2018, 678, 169-176.	0.8	5
1133	First-principles studies of SnS2, MoS2 and WS2 stacked van der Waals hetero-multilayers. Computational Condensed Matter, 2018, 16, e00303.	0.9	5
1134	Controlling Band Alignment in Molecular Junctions: Utilizing Two-Dimensional Transition-Metal Dichalcogenides as Electrodes for Thermoelectric Devices. Journal of Physical Chemistry C, 2018, 122, 14233-14239.	1.5	11
1135	Van der Waals interactions and the properties of graphite and 2H-, 3R- and 1T-MoS2: A comparative study. Computational Materials Science, 2018, 152, 146-150.	1.4	30
1136	Influence of graphene thickness and grain boundaries on MoS₂ wrinkle nanostructures. Physical Chemistry Chemical Physics, 2018, 20, 17000-17008.	1.3	9
1137	DFT studies on storage and adsorption capacities of gases on MOFs. Physical Sciences Reviews, 2018, 3, .	0.8	2
1138	On the diversity in the thermal transport properties of graphene: A first-principles-benchmark study testing different exchange-correlation functionals. Computational Materials Science, 2018, 151, 153-159.	1.4	34
1139	Field-induced structural control of COx molecules adsorbed on graphene. Journal of Applied Physics, 2018, 123, 174302.	1.1	1
1140	Computational findings of metastable ferroelectric phases of squaric acid. Physical Review B, 2018, 97, .	1.1	17
1141	Assessment of Density Functional Methods for Geometry Optimization of Bimolecular van der Waals Complexes. Journal of Chemical Theory and Computation, 2018, 14, 3004-3013.	2.3	27
1142	Phase Diagram of Methane Hydrates and Discovery of MH-VI Hydrate. Journal of Physical Chemistry A, 2018, 122, 6007-6013.	1.1	5
1143	Influence of Tight Confinement on Selective Oxidative Dehydrogenation of Ethane on MoVTeNb Mixed Oxides. ACS Catalysis, 2018, 8, 7051-7067.	5.5	59

#	Article	IF	Citations
1144	A dispersion-corrected DFT investigation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="italic">CH</mml:mi></mml:mrow><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:m adsorption by silver-decorated monolayer graphene in the presence of ambient oxygen molecules. Applied Surface Science, 2018, 457, 303-314.	3.1	35
1145	Electronic Structure of a Polybenzimidazole-Wrapped Single-Wall Carbon Nanotube. Journal of Physical Chemistry C, 2018, 122, 15979-15985.	1.5	7
1146	Ab initio design of light absorption through silver atomic cluster decoration of TiO₂. Physical Chemistry Chemical Physics, 2018, 20, 19110-19119.	1.3	31
1147	Prediction of a metallic phase for Cs3Pentacene compound. Materials Research Express, 2018, 5, 066554.	0.8	2
1148	Dynamics of N2 sticking on W(100): the decisive role of van der Waals interactions. Physical Chemistry Chemical Physics, 2018, 20, 19326-19331.	1.3	10
1149	Role of Surface Hydroxyl Species in Copper-Catalyzed Hydrogenation of Ketones. ACS Catalysis, 2018, 8, 7539-7548.	5.5	35
1150	SnP₃: A Previously Unexplored Two-Dimensional Material. Journal of Physical Chemistry C, 2018, 122, 18185-18191.	1.5	85
1151	Coarse-Grained Double-Stranded RNA Model from Quantum-Mechanical Calculations. Journal of Physical Chemistry B, 2018, 122, 7915-7928.	1.2	10
1152	Combining Wave Function Methods with Density Functional Theory for Excited States. Chemical Reviews, 2018, 118, 7249-7292.	23.0	166
1153	Geometry optimisations with a nonlocal density-functional theory method based on a double Hirshfeld partitioning. Journal of Chemical Physics, 2018, 149, 044103.	1.2	2
1154	Computational screening of organic polymer dielectrics for novel accelerator technologies. Scientific Reports, 2018, 8, 9258.	1.6	4
1155	Role of Stone-Wales defects on the interfacial interactions among graphene, carbon nanotubes, and Nylon 6: A first-principles study. Journal of Chemical Physics, 2018, 149, 054703.	1.2	11
1156	Tailoring van der Waals dispersion interactions with external electric charges. Nature Communications, 2018, 9, 3017.	5.8	23
1157	Magnetic Transitions in K-Doped Biphenyl and ${p}$ -Terphenyl. IEEE Transactions on Magnetics, 2018, 54, 1-5.	1.2	3
1158	Lithium Borocarbide LiBC as an Anode Material for Rechargeable Li-Ion Batteries. Journal of Physical Chemistry C, 2018, 122, 18231-18236.	1.5	16
1159	Structural evolution of gypsum under high pressure: single-crystal X-ray experiments revisited. Physics and Chemistry of Minerals, 2018, 45, 895-906.	0.3	2
1160	Nanoscale surface dynamics of Bi₂Te₃(111): observation of a prominent surface acoustic wave and the role of van der Waals interactions. Nanoscale, 2018, 10, 14627-14636.	2.8	27
1161	Elastic properties of bulk and low-dimensional materials using van der Waals density functional. Physical Review B, 2018, 98, .	1.1	88

#	Article	IF	Citations
1162	Unusual Pressure-Induced Periodic Lattice Distortion in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>SnSe</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></ Physical Review Letters, 2018, 121, 027003.	2.9	24
1163	Van der Waals Density Functional Theory Study of Molecular Adsorbates on MoX2(X = S, Se or Te). Journal of the Korean Physical Society, 2018, 73, 100-104.	0.3	14
1164	Toward a Reliable Description of the Lattice Vibrations in Organic Molecular Crystals: The Impact of van der Waals Interactions. Journal of Chemical Theory and Computation, 2018, 14, 4380-4390.	2.3	26
1165	Predicted Binary Compounds of Tin and Sulfur. Journal of Physical Chemistry C, 2018, 122, 17067-17072.	1.5	6
1166	A dispersion-corrected DFT insight into the structural, electronic and CH4 adsorption properties of small tin-oxide clusters. Journal of Alloys and Compounds, 2018, 757, 382-392.	2.8	8
1167	Revealing the formation and electrochemical properties of bis(trifluoromethanesulfonyl)imide intercalated graphite with first-principles calculations. Physical Chemistry Chemical Physics, 2018, 20, 14124-14132.	1.3	19
1168	Benchmarking of GGA density functionals for modeling structures of nanoporous, rigid and flexible MOFs. Journal of Chemical Physics, 2018, 149, 064110.	1.2	23
1169	Phase stability and interlayer interaction of blue phosphorene. Physical Review B, 2018, 98, .	1.1	19
1170	A topologically substituted boron nitride hybrid aerogel for highly selective CO2 uptake. Nano Research, 2018, 11, 6325-6335.	5.8	14
1171	Distinct Differences in Peptide Adsorption on Palladium and Gold: Introducing a Polarizable Model for Pd(111). Journal of Physical Chemistry C, 2018, 122, 19625-19638.	1.5	7
1172	Accelerated discovery of stable lead-free hybrid organic-inorganic perovskites via machine learning. Nature Communications, 2018, 9, 3405.	5.8	442
1173	Probing the chirality-dependent elastic properties and crack propagation behavior of single and bilayer stanene. Physical Chemistry Chemical Physics, 2018, 20, 22768-22782.	1.3	27
1174	Rational design of new phases of tin monosulfide by first-principles structure searches. Science China: Physics, Mechanics and Astronomy, 2018, 61, 1.	2.0	15
1175	Light-Activated Hybrid Nanocomposite Film for Water and Oxygen Sensing. ACS Applied Materials & Interfaces, 2018, 10, 31745-31754.	4.0	12
1176	Energetics and electronic structures of perylene confined in carbon nanotubes. Royal Society Open Science, 2018, 5, 180359.	1.1	2
1177	Insulator-metal transition in dense fluid deuterium. Science, 2018, 361, 677-682.	6.0	108
1178	MoirÃ© Phonons in Twisted Bilayer MoS₂. ACS Nano, 2018, 12, 8770-8780.	7.3	149
1179	The evolution in graphitic surface wettability with first-principles quantum simulations: the counterintuitive role of water. Physical Chemistry Chemical Physics, 2018, 20, 22636-22644.	1.3	23

#	Article	IF	Citations
1180	Quantum anomalous Hall effect in metal-bis(dithiolene), magnetic properties, doping and interfacing graphene. Physical Chemistry Chemical Physics, 2018, 20, 22652-22659.	1.3	14
1181	The adsorption of alcohols on strained Pt₃Ni(111) substrates: a density functional investigation within the D3 van der Waals correction. Physical Chemistry Chemical Physics, 2018, 20, 24210-24221.	1.3	14
1182	Comparative study of structural and electronic properties of GaSe and InSe polytypes. Journal of Chemical Physics, 2018, 149, 054106.	1.2	35
1183	Computational Understanding of the Growth of 2D Materials. Advanced Theory and Simulations, 2018, 1, 1800085.	1.3	30
1184	Modeling and measurements of the XRD patterns of extended solids under high-pressure. AIP Conference Proceedings, 2018, , .	0.3	3
1185	Few-Layer PdSe₂ Sheets: Promising Thermoelectric Materials Driven by High Valley Convergence. ACS Omega, 2018, 3, 5971-5979.	1.6	87
1186	Water agglomerates on Fe ₃ O ₄ (001). Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E5642-E5650.	3.3	79
1187	Mapping uncharted territory in iceÂfrom zeolite networks to ice structures. Nature Communications, 2018, 9, 2173.	5.8	57
1188	Diffusion quantum Monte Carlo and density functional calculations of the structural stability of bilayer arsenene. Journal of Chemical Physics, 2018, 148, 214706.	1.2	23
1189	Computational Study on Atomic Structures, Electronic Properties, and Chemical Reactions at Surfaces and Interfaces and in Biomaterials. Journal of the Physical Society of Japan, 2018, 87, 061013.	0.7	2
1190	Factors driving stable growth of He clusters in W: first-principles study. Nuclear Fusion, 2018, 58, 076024.	1.6	2
1191	Predicting vapor liquid equilibria using density functional theory: A case study of argon. Journal of Chemical Physics, 2018, 148, 224501.	1.2	10
1192	New Model for Predicting Adsorption of Polar Molecules in Metalâ€“Organic Frameworks with Unsaturated Metal Sites. Journal of Physical Chemistry Letters, 2018, 9, 3544-3553.	2.1	29
1193	Theoretical Investigation of Metallic Nanolayers For Charge-Storage Applications. ACS Applied Energy Materials, 2018, 1, 3428-3433.	2.5	19
1194	Ab initio density functional theory study of the electronic, dynamic, and thermoelectric properties of the crystalline pseudobinary chalcogenide <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mtext>(GeTe)</mml:mtext></mml:mrow><mml width="0.. Physical Review B, 2018, 97, .	1.1	18
1195	Quasicrystalline 30Â° twisted bilayer graphene as an incommensurate superlattice with strong interlayer coupling. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6928-6933.	3.3	169
1196	Quantitative diagnostics of ancient paper using THz time-domain spectroscopy. Microchemical Journal, 2018, 142, 54-61.	2.3	9
1197	Helium and Argon Interactions with Gold Surfaces: Ab Initio-Assisted Determination of the Heâ€“Au Pairwise Potential and Its Application to Accommodation Coefficient Determination. Journal of Physical Chemistry C, 2018, 122, 14606-14614.	1.5	7

#	Article	IF	Citations
1198	A Monolayer of Hexagonal Boron Nitride on Ir(111) as a Template for Cluster Superlattices. ACS Nano, 2018, 12, 6871-6880.	7.3	31
1199	Nanomechanics of graphene. National Science Review, 2019, 6, 324-348.	4.6	75
1200	First principles-based multiscale atomistic methods for input into first principles nonequilibrium transport across interfaces. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 18193-18201.	3.3	7
1201	Highâ€tthroughput computational screening of layered and twoâ€dimensional materials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1385.	6.2	43
1202	Adverse effects of interlayer-gliding in layered transition-metal oxides on electrochemical sodium-ion storage. Energy and Environmental Science, 2019, 12, 825-840.	15.6	205
1203	Dissociative Chemisorption of Methane on Stepped Ir(332) Surface: Density Functional Theory and Ab Initio Molecular Dynamics Studies. Journal of Physical Chemistry C, 2019, 123, 20893-20902.	1.5	12
1204	Electronic and optical properties of GaNâ€“MoS₂ heterostructure from first-principles calculations*. Chinese Physics B, 2019, 28, 086104.	0.7	9
1205	Electron Density Studies in Materials Research. Chemistry - A European Journal, 2019, 25, 15010-15029.	1.7	26
1206	Adsorption on transition metal surfaces: Transferability and accuracy of DFT using the ADS41 dataset. Physical Review B, 2019, 100, .	1.1	51
1207	Deuterium Hugoniot: Pitfalls of thermodynamic sampling beyond density functional theory. Physical Review B, 2019, 100, .	1.1	7
1208	Large Nontrivial Topological Band Gap in Heterostructure of Fluorine-Functionalized Bismuthene and h-BN Substrate: A First Principles Study. , 2019, , .		1
1209	Influence of Local Defects on the Dynamics of Oâ€“H Bond Breaking and Formation on a Magnetite Surface. Journal of Physical Chemistry C, 2019, 123, 19742-19747.	1.5	11
1210	Nonoxidative Direct Conversion of Methane on Silica-Based Iron Catalysts: Effect of Catalytic Surface. ACS Catalysis, 2019, 9, 7984-7997.	5.5	61
1211	Shape of Cobalt and Platinum Nanoparticles Under a CO Atmosphere: A Combined In Situ TEM and Computational Catalysis Study. ACS Catalysis, 2019, 9, 7449-7456.	5.5	21
1212	Single-atom Fe and N co-doped graphene for lithium-sulfur batteries: a density functional theory study. Materials Research Express, 2019, 6, 095620.	0.8	29
1213	Fabrication of large-scale graphene/2D-germanium heterostructure by intercalation. Chinese Physics B, 2019, 28, 078103.	0.7	6
1214	Axial field induced spin response in Fe/hBN-based tunnel junctions. Physical Review B, 2019, 100, .	1.1	5
1215	Suppressing Xâ€Migrations and Enhancing the Phase Stability of Cubic FAPbX₃ (X = Br, I). Advanced Energy Materials, 2019, 9, 1901411.	10.2	20

#	Article	IF	Citations
1216	Local Structure and Coordination Define Adsorption in a Model Ir₁/Fe₃O₄ Singleâ€Atom Catalyst. Angewandte Chemie - International Edition, 2019, 58, 13961-13968.	7.2	93
1217	Local Structure and Coordination Define Adsorption in a Model Ir₁/Fe₃O₄ Singleâ€Atom Catalyst. Angewandte Chemie, 2019, 131, 14099-14106.	1.6	44
1218	Water Enables Efficient CO₂ Capture from Natural Gas Flue Emissions in an Oxidation-Resistant Diamine-Appended Metalâ€“Organic Framework. Journal of the American Chemical Society, 2019, 141, 13171-13186.	6.6	107
1219	Toward a Specific Reaction Parameter Density Functional for H2 + Ni(111): Comparison of Theory with Molecular Beam Sticking Experiments. Journal of Physical Chemistry C, 2019, 123, 20420-20433.	1.5	12
1220	Crystal Structures and Energy Storage Properties of Ammine Sodium Decahydro-closo-decaboranes (Na2B10H10Â·nNH3, n = 1, 2). Journal of Physical Chemistry C, 2019, 123, 20160-20166.	1.5	10
1221	Autocatalytic Role of Molecular Hydrogen in Copper-Catalyzed Transfer Hydrogenation of Ketones. ACS Catalysis, 2019, 9, 8073-8082.	5.5	16
1222	Electronic Structure and Theoretical Aspects on Sensing Application of 2D Materials. , 2019, , 145-203.		7
1223	Exchange-correlation thermal effects in shocked deuterium: Softening the principal Hugoniot and thermophysical properties. Physical Review B, 2019, 99, .	1.1	22
1224	Enhanced Photo-Electrocatalytic Hydrogen Generation in Graphene/hBN van der Waals Structures. Journal of Physical Chemistry C, 2019, 123, 17249-17254.	1.5	6
1225	Prominent out-of-plane diffraction in helium scattering from a methyl-terminated Si(111) surface. Physical Chemistry Chemical Physics, 2019, 21, 15879-15887.	1.3	2
1226	Probing DNA nucleobases with diamond (111) surfaces. Journal of Physics Communications, 2019, 3, 095007.	0.5	0
1227	Structure, Dynamics, and Wettability of Water at Metal Interfaces. Scientific Reports, 2019, 9, 14805.	1.6	38
1228	Structural and electronic properties of liquid, amorphous, and supercooled liquid phases of In2Te5 from first-principles. Journal of Chemical Physics, 2019, 151, 134503.	1.2	8
1229	Adsorption of NO Gas Molecules on Monolayer Arsenene Doped with Al, B, S and Si: A First-Principles Study. Processes, 2019, 7, 538.	1.3	8
1230	Tunable Schottky and Ohmic contacts in graphene and tellurene van der Waals heterostructures. Physical Chemistry Chemical Physics, 2019, 21, 23611-23619.	1.3	24
1231	Nanotribological Properties of the h-BN/Au(111) Interface: A DFT Study. Journal of Physical Chemistry C, 2019, 123, 28411-28418.	1.5	10
1234	Performance of Taoâ€“Mo Semilocal Functional with rVV10 Dispersion-Correction: Influence of Different Correlation. Journal of Physical Chemistry A, 2019, 123, 10582-10593.	1.1	14
1235	The Equation of State of MH-III: A Possible Deep CH₄ Reservoir in Titan, Super-Titan Exoplanets, and Moons. Astrophysical Journal, 2019, 882, 71.	1.6	6

#	Article	IF	Citations
1236	Relative Abundance of Z2 Topological Order in Exfoliable Two-Dimensional Insulators. Nano Letters, 2019, 19, 8431-8440.	4.5	50
1237	Phonon dynamics in the layered negative thermal expansion compounds CuxNi2â^'x(CN)4. Physical Review B, 2019, 100, .	1.1	9
1238	Interaction between water and carbon nanostructures: How good are current density functional approximations?. Journal of Chemical Physics, 2019, 151, 164702.	1.2	47
1239	A study of properties of palladium metal as a component of fuel cells. Materials Research Express, 2019, 6, 105540.	0.8	7
1240	Theoretical prediction of superconductivity in monolayer CoO2. Nanoscale, 2019, 11, 17052-17057.	2.8	9
1241	Morphology and Electronic Structure of Sn-Intercalated TiS2(0001) Layers. Journal of Physical Chemistry C, 2019, 123, 22293-22298.	1.5	6
1242	Photochemically Induced Water Harvesting in Metalâ€“Organic Framework. ACS Sustainable Chemistry and Engineering, 2019, 7, 15854-15859.	3.2	24
1243	Out-of-plane ion transport makes nitrogenated holey graphite a promising high-rate anode for both Li and Na ion batteries. Nanoscale, 2019, 11, 18758-18768.	2.8	22
1244	What Is the Best Size of Subnanometer Copper Clusters for CO₂ Conversion to Methanol at Cu/TiO₂ Interfaces? A Density Functional Theory Study. Journal of Physical Chemistry C, 2019, 123, 24118-24132.	1.5	32
1245	Assessment of van der Waals inclusive density functional theory methods for adsorption and selective dehydrogenation of formic acid on Pt(111) surface. Physical Chemistry Chemical Physics, 2019, 21, 21049-21056.	1.3	23
1246	Molecular Dynamics Study of the Effect of <scp>l</scp>-Alanine Chiral Dopants on Diluted Chromonic Solutions. Journal of Physical Chemistry B, 2019, 123, 8995-9010.	1.2	6
1247	Diffusion Monte Carlo study of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> adsorption on single layer graphene. Physical Review B, 2019, 100, .	1.1	6
1248	Rationally Designed High-Performance Spin Filter Based on Two-Dimensional Half-Metal Cr2NO2. Matter, 2019, 1, 1304-1315.	5.0	30
1249	The role of H₂S addition on Pt/Al₂O₃ catalyzed propane dehydrogenation: a mechanistic study. Catalysis Science and Technology, 2019, 9, 867-876.	2.1	21
1250	Priming effects in the crystallization of the phase change compound GeTe from atomistic simulations. Faraday Discussions, 2019, 213, 287-301.	1.6	18
1251	Strong interfacial interactions induced a large reduction in lateral thermal conductivity of transition-metal dichalcogenide superlattices. RSC Advances, 2019, 9, 1387-1393.	1.7	7
1252	A hypervalent and cubically coordinated molecular phase of IF₈predicted at high pressure. Chemical Science, 2019, 10, 2543-2550.	3.7	36
1253	Lattice dynamics and negative thermal expansion in the framework compound <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>ZnNi</mml:mi><mml:msub><mml:mrow><mml:mo>(</mml:mo> with two-dimensional and three-dimensional local environments. Physical Review B, 2019, 99, .	1.1	26

#	Article	IF	Citations
1254	Implementation of the Many-Pair Expansion for Systematically Improving Density Functional Calculations of Molecules. Journal of Chemical Theory and Computation, 2019, 15, 1089-1101.	2.3	5
1255	Effects of Sodium and Magnesium Cations on the Aggregation of Chromonic Solutions Using Molecular Dynamics. Journal of Physical Chemistry B, 2019, 123, 1718-1732.	1.2	9
1256	Liquids with Lower Wettability Can Exhibit Higher Friction on Hexagonal Boron Nitride: The Intriguing Role of Solidâ€“Liquid Electrostatic Interactions. Nano Letters, 2019, 19, 1539-1551.	4.5	39
1257	Origin of the Immiscibility of Alkanes and Perfluoroalkanes. Journal of the American Chemical Society, 2019, 141, 3489-3506.	6.6	45
1258	Engineering Point-Defect States in Monolayer WSe₂. ACS Nano, 2019, 13, 1595-1602.	7.3	35
1259	Alkaliâ€Metalâ€Intercalated Percolation Network Regulates Selfâ€Assembled Electronic Aromatic Molecules. Advanced Materials, 2019, 31, e1807178.	11.1	11
1260	Theoretical Design of Layered AlGaS3 as a New Nonlinear Optical Material with a Strong Second Harmonic Generation Response. Crystal Growth and Design, 2019, 19, 1632-1639.	1.4	1
1261	Polar Metallocenes. Molecules, 2019, 24, 486.	1.7	1
1262	Energy Dissipation Effects on the Adsorption Dynamics of N2 on W(100). Journal of Physical Chemistry C, 2019, 123, 2900-2910.	1.5	5
1263	Tuning the electronic and magnetic properties of metal-doped phenanthrene by codoping method. AIP Advances, 2019, 9, .	0.6	2
1264	Mechanical Properties of Formamidinium Halide Perovskites FABX₃ (FA=CH(NH₂)₂; B=Pb, Sn; X=Br, I) by First-Principles Calculations[*]. Chinese Physics Letters, 2019, 36, 056201.	1.3	33
1265	Layertronic control of topological states in multilayer metal-organic frameworks. Journal of Chemical Physics, 2019, 150, 234701.	1.2	15
1266	Structural correlations tailor conductive properties in polymerized ionic liquids. Physical Chemistry Chemical Physics, 2019, 21, 14775-14785.	1.3	9
1267	The purported square ice in bilayer graphene is a nanoscale, monolayer object. Journal of Chemical Physics, 2019, 150, 231101.	1.2	7
1268	Disparate strain response of the thermal transport properties of bilayer penta-graphene as compared to that of monolayer penta-graphene. Physical Chemistry Chemical Physics, 2019, 21, 15647-15655.	1.3	28
1269	Phthalocyanine and Metal Phthalocyanines Adsorbed on Graphene: A Density Functional Study. Journal of Physical Chemistry C, 2019, 123, 16614-16620.	1.5	33
1270	A theoretical approach of the ethanol adsorption on Au(100), Au(110) and Au(111) surfaces. Surface Science, 2019, 689, 121458.	0.8	5
1271	Impact of Stoichiometry and Fluorine Atoms on the Charge Transport of Peryleneâ€“F₄TCNQ. Journal of Physical Chemistry Letters, 2019, 10, 3376-3380.	2.1	15

#	Article	IF	Citations
1272	Asymmetric carrier accumulation in van der Waals heterostructures of MoS2/WS2 under an external electric field. Applied Physics Express, 2019, 12, 075008.	1.1	10
1273	Specific Reaction Parameter Density Functional Based on the Meta-Generalized Gradient Approximation: Application to H₂ + Cu(111) and H₂ + Ag(111). Journal of Physical Chemistry A, 2019, 123, 5395-5406.	1.1	28
1274	Stepwise on-surface dissymmetric reaction to construct binodal organometallic network. Nature Communications, 2019, 10, 2545.	5.8	26
1275	Dispersion Energy from Local Polarizability Density. Physical Review Letters, 2019, 122, 213001.	2.9	11
1276	Interfacial properties of water/heavy water layer encapsulate in bilayer graphene nanochannel and nanocapacitor. Journal of Materials Science: Materials in Electronics, 2019, 30, 11964-11975.	1.1	2
1277	Commensurate-incommensurate phase transition and a network of domain walls in bilayer graphene with a biaxially stretched layer. Physical Review B, 2019, 99, .	1.1	19
1278	Connecting Solution-Phase to Single-Molecule Properties of Ni(Salophen). Journal of Physical Chemistry Letters, 2019, 10, 3525-3530.	2.1	8
1279	Equipartition of Energy Defines the Sizeâ€“Thickness Relationship in Liquid-Exfoliated Nanosheets. ACS Nano, 2019, 13, 7050-7061.	7.3	123
1280	First-order liquid-liquid phase transition in compressed hydrogen and critical point. Journal of Chemical Physics, 2019, 150, 204114.	1.2	6
1281	Towards reliable ab initio sublimation pressures for organic molecular crystals â€“ are we there yet?. Physical Chemistry Chemical Physics, 2019, 21, 14799-14810.	1.3	17
1282	An ultralow-density porous ice with the largest internal cavity identified in the water phase diagram. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 12684-12691.	3.3	16
1283	Computational discovery of nanoporous materials for energy- and environment-related applications. Molecular Simulation, 2019, 45, 1122-1147.	0.9	23
1284	A DFTâ€¯+â€¯U study of H2O adsorption on the V2O5(0 0 1) surface including van der Waals interactions. Chemical Physics Letters, 2019, 730, 171-178.	1.2	7
1285	Theory and practice of modeling van der Waals interactions in electronic-structure calculations. Chemical Society Reviews, 2019, 48, 4118-4154.	18.7	114
1286	Ab Initio Search of Polymer Crystals with High Thermal Conductivity. Chemistry of Materials, 2019, 31, 4649-4656.	3.2	9
1287	Automated Detection and Characterization of Surface Restructuring Events in Bimetallic Catalysts. Journal of Physical Chemistry C, 2019, 123, 16332-16344.	1.5	10
1288	Domain wall pinning and hard magnetic phase in Co-doped bulk single crystalline <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>13</mml:mn></mml:msub></mml:r Physical Review B, 2019, 99, .	1.1	53
1289	Gold(<scp>i</scp>) sulfide: unusual bonding and an unexpected computational challenge in a simple solid. Chemical Science, 2019, 10, 6467-6475.	3.7	12

#	Article	IF	Citations
1290	UV-SWIR broad range photodetectors made from few-layer Î±-In₂Se₃ nanosheets. Nanoscale, 2019, 11, 12817-12828.	2.8	47
1291	Energetics and structure of Langmuir monolayers of palmitic acid: a DFT study. Physical Chemistry Chemical Physics, 2019, 21, 11203-11213.	1.3	5
1292	van der Waals density functional with corrected <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>C</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:m coefficients. Physical Review B, 2019, 99, .	1.1	12
1293	Formaldehyde adsorption on a hydrogenated aluminum nitride monolayer: A self-propagated reaction. Computational and Theoretical Chemistry, 2019, 1159, 18-22.	1.1	8
1294	Alloy structure of rare earth Ce with Pt base metal, and the adsorption of CO. Materials Research Express, 2019, 6, 046538.	0.8	0
1295	Van der Waals Density Functional Theory vdW-DFq for Semihard Materials. Crystals, 2019, 9, 243.	1.0	22
1296	General adsorption model for H2S, H2Se, H2Te, NH3, PH3, AsH3 and SbH3 on the V2O5(0 0 1) surface including the van der Waals interaction. Chemical Physics Letters, 2019, 720, 58-63.	1.2	30
1297	Phonon dispersion in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></ Physical Review B, 2019, 99, .	1.1	49
1298	Computational Design of Mixed-Valence Tin Sulfides as Solar Absorbers. ACS Applied Materials & Interfaces, 2019, 11, 24867-24875.	4.0	11
1299	Analysis of the fluorescence of mechanically processed defect-laden hexagonal boron nitride and the role of oxygen in catalyst deactivation. Advances in Applied Ceramics, 2019, 118, 153-158.	0.6	5
1300	Photovoltaic Performance of Lead-Less Hybrid Perovskites from Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 12638-12646.	1.5	39
1301	Adsorption and dissociation of iron phthalocyanine on H/Si(111): Impact of van der Waals interactions and perspectives for subsurface doping. Physical Review B, 2019, 99, .	1.1	6
1302	Electronic properties and interlayer coupling of twisted <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub><mm heterobilayers. Physical Review B, 2019, 99, .	1.1	28
1303	Full orientation control of epitaxial <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></ on hBN assisted by substrate defects. Physical Review B, 2019, 99, .	1.1	37
1304	Layer breathing and shear modes in multilayer graphene: a DFT-vdW study. Journal of Physics Condensed Matter, 2019, 31, 295301.	0.7	5
1305	Metastable molecular fluid hydrogen at high pressures. Contributions To Plasma Physics, 2019, 59, e201800173.	0.5	6
1306	Room temperature electrofreezing of water yields a missing dense ice phase in the phase diagram. Nature Communications, 2019, 10, 1925.	5.8	20
1307	van der Waals interactions in DFT using Wannier functions without empirical parameters. Journal of Chemical Physics, 2019, 150, 164109.	1.2	14

#	Article	IF	Citations
1308	How far does the defect tolerance of lead-halide perovskites range? The example of Bi impurities introducing efficient recombination centers. Journal of Materials Chemistry A, 2019, 7, 23838-23853.	5.2	57
1309	Role of Ketoâ€“Enol Tautomerization in the Copper-Catalyzed Hydrogenation of Ketones. ACS Catalysis, 2019, 9, 3831-3839.	5.5	17
1310	Role of Metal Centers in Tuning the Electronic Properties of Graphene-Based Conductive Interfaces. Journal of Physical Chemistry C, 2019, 123, 8623-8632.	1.5	11
1311	Protection of one-dimensional Si chains embedded in Pt(111) and protected by a hexagonal boron-nitride monolayer. Surface Science, 2019, 685, 24-33.	0.8	0
1312	Li and Na Adsorption on Graphene and Graphene Oxide Examined by Density Functional Theory, Quantum Theory of Atoms in Molecules, and Electron Localization Function. Molecules, 2019, 24, 754.	1.7	39
1313	Amphoteric behavior of hydrogen (H⁺¹ and H^{â^'1}) in complex hydrides from van der Waals interaction-including ab initio calculations. Journal of Materials Chemistry A, 2019, 7, 6228-6240.	5.2	7
1314	A New Equation of State for Dense Hydrogenâ€“Helium Mixtures. Astrophysical Journal, 2019, 872, 51.	1.6	99
1315	Assessment of Density Functional Theory in Predicting Interaction Energies between Water and Polycyclic Aromatic Hydrocarbons: from Water on Benzene to Water on Graphene. Journal of Chemical Theory and Computation, 2019, 15, 2359-2374.	2.3	18
1316	BEEF-vdW+U method applied to perovskites: thermodynamic, structural, electronic, and magnetic properties. Journal of Physics Condensed Matter, 2019, 31, 145901.	0.7	11
1317	Assessment of Two Problems of Specific Reaction Parameter Density Functional Theory: Sticking and Diffraction of H₂ on Pt(111). Journal of Physical Chemistry C, 2019, 123, 10406-10418.	1.5	10
1318	Structural and Electronic Properties of Double-Walled Black Phosphorene Nanotubes: A Density Functional Theory Study. Journal of Physical Chemistry C, 2019, 123, 7217-7224.	1.5	12
1319	Benchmarking the performance of approximate van der Waals methods for the structural and energetic properties of SiO2 and AlPO4 frameworks. Journal of Chemical Physics, 2019, 150, 094102.	1.2	24
1320	Boosting Rechargeable Batteries R&D by Multiscale Modeling: Myth or Reality?. Chemical Reviews, 2019, 119, 4569-4627.	23.0	204
1321	Raman detection of hidden phonons assisted by atomic point defects in a two-dimensional semimetal. Npj 2D Materials and Applications, 2019, 3, .	3.9	10
1322	Scanning tunneling microscopy and Raman evidence of silicene nanosheets intercalated into graphite surfaces at room temperature. Nanoscale, 2019, 11, 6145-6152.	2.8	14
1323	The effect of Fe vacancies and Cu adhesion on the magnetic properties of Fe₃GeTe₂. Physical Chemistry Chemical Physics, 2019, 21, 7588-7593.	1.3	11
1324	Unraveling the Potassium Storage Mechanism in Graphite Foam. Advanced Energy Materials, 2019, 9, 1900579.	10.2	133
1325	Electronic properties of h-BN/g-C2N van der Waals heterojunction: A first-principles calculation. Chemical Physics Letters, 2019, 725, 75-79.	1.2	12

#	Article	IF	Citations
1326	Dual effect of humidity on cesium lead bromide: enhancement and degradation of perovskite films. Journal of Materials Chemistry A, 2019, 7, 12292-12302.	5.2	74
1327	Improved DFT Adsorption Energies with Semiempirical Dispersion Corrections. Journal of Chemical Theory and Computation, 2019, 15, 3250-3259.	2.3	43
1328	Exploration of Long-Life Pt/Heteroatom-Doped Graphene Catalysts in Hydrogen Atmosphere. ACS Omega, 2019, 4, 6573-6584.	1.6	2
1329	van der Waals exchange-correlation functionals over bulk and surface properties of transition metals. Journal of Physics Condensed Matter, 2019, 31, 315501.	0.7	10
1330	Structure, charge transfer, and superconductivity of M-doped phenanthrene (M = Al, Ga, and In): A comparative study of K-doped cases. Science China: Physics, Mechanics and Astronomy, 2019, 62, 1.	2.0	4
1331	Ab initio calculations and reduced density gradient analyses of the structure and energetics of hydrated calcium fluoride and calcium carbonate. Physical Chemistry Chemical Physics, 2019, 21, 5744-5758.	1.3	5
1332	A family of high-temperature ferromagnetic monolayers with locked spin-dichroism-mobility anisotropy: MnNX and CrCX (Xâ€¯=â€¯Cl, Br, I; Câ€¯=â€¯S, Se, Te). Science Bulletin, 2019, 64, 293-300.	4.3	96
1333	Uncertainty Quantification in First-Principles Predictions of Harmonic Vibrational Frequencies of Molecules and Molecular Complexes. Journal of Physical Chemistry C, 2019, 123, 4072-4084.	1.5	16
1334	Coordination-Controlled Câ€“C Coupling Products via ortho-Site Câ€“H Activation. ACS Nano, 2019, 13, 1385-1393.	7.3	25
1335	Restructuring of MFI Framework Zeolite Models and Their Associated Artifacts in Density Functional Theory Calculations. Journal of Physical Chemistry C, 2019, 123, 6572-6585.	1.5	21
1336	Multi Band Gap Electronic Structure in CH3NH3PbI3. Scientific Reports, 2019, 9, 2144.	1.6	26
1337	Wet Chemical Method for Black Phosphorus Thinning and Passivation. ACS Applied Materials & Interfaces, 2019, 11, 9213-9222.	4.0	23
1338	From DFT to machine learning: recent approaches to materials scienceâ€“a review. JPhys Materials, 2019, 2, 032001.	1.8	385
1339	A Trip to the Density Functional Theory Zoo: Warnings and Recommendations for the User. Australian Journal of Chemistry, 2019, 72, 563.	0.5	115
1340	Combined effect of point defects and layer number on the adsorption of benzene and toluene on graphene. Applied Surface Science, 2019, 480, 1063-1069.	3.1	12
1341	Strongly Correlated Aromatic Molecular Conductor. Small, 2019, 15, e1900299.	5.2	4
1342	Influence of nanotube section on carboplatin confinement. Journal of Molecular Modeling, 2019, 25, 72.	0.8	7
1343	Water Splitting Reaction at Polar Lithium Niobate Surfaces. ACS Omega, 2019, 4, 3850-3859.	1.6	16

#	Article	IF	Citations
1344	Biogas detection on carbon nitride sheet with embedded Mn atom: dispersion-corrected density functional theory. Materials Research Express, 2019, 6, 065603.	0.8	4
1345	Ignition of discharges in macroscopic isolated voids and first electron availability. Journal of Applied Physics, 2019, 125, .	1.1	13
1346	Phonons in deformable microporous crystalline solids. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 513-527.	0.4	7
1347	Direct Vapor Growth of 2D Vertical Heterostructures with Tunable Band Alignments and Interfacial Charge Transfer Behaviors. Advanced Science, 2019, 6, 1802204.	5.6	87
1348	Towards the Same Line of Liquidâ€“Liquid Phase Transition of Dense Hydrogen from Various Theoretical Predictions[*]. Chinese Physics Letters, 2019, 36, 103102.	1.3	15
1349	Gap opening in the most stable phases of K₃ Terphenyl compound. Materials Research Express, 2019, 6, 125111.	0.8	1
1350	Superconducting Single-Layer T-Graphene and Novel Synthesis Routes*. Chinese Physics Letters, 2019, 36, 097401.	1.3	61
1351	Effects of Lattice O Atom Coordination and Pore Confinement on Selectivity Limitations for Ethane Oxidative Dehydrogenation Catalyzed by Vanadium-Oxo Species. Journal of Physical Chemistry C, 2019, 123, 28168-28191.	1.5	20
1352	Ensemble first-principles molecular dynamics simulations of water using the SCAN meta-GGA density functional. Journal of Chemical Physics, 2019, 151, 164101.	1.2	24
1353	First-Principles Study of Alkyl Derivatives of Boehmite. Journal of the Korean Physical Society, 2019, 75, 490-493.	0.3	1
1354	In search of the most active MN4 catalyst for the oxygen reduction reaction. The case of perfluorinated Fe phthalocyanine. Journal of Materials Chemistry A, 2019, 7, 24776-24783.	5.2	52
1355	Trends of the macroscopic behaviors of energetic compounds: insights from first-principles calculations. Physical Chemistry Chemical Physics, 2019, 21, 24034-24041.	1.3	3
1356	Monolayer SnP₃: an excellent p-type thermoelectric material. Nanoscale, 2019, 11, 19923-19932.	2.8	119
1357	Uncertainty quantification of DFT-predicted finite temperature thermodynamic properties within the Debye model. Journal of Chemical Physics, 2019, 151, 244702.	1.2	13
1358	Prediction of room-temperature half-metallicity in layered halide double perovskites. Npj Computational Materials, 2019, 5, .	3.5	19
1359	Six-dimensional potential energy surfaces for the dissociative chemisorption of HCl on rigid Ag(100) and Ag(110) surfaces. Journal of Chemical Physics, 2019, 151, 144707.	1.2	10
1360	Anomalous thermal expansion in one-dimensional transition metal cyanides: Behavior of the trimetallic cyanide <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">u</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>/</mml:mo><mml:mn>3</mml:mn></mml:mrow></r mathvariant="normal">A</mml:mi><mml:msub><mml:mi mathvariant="normal">g</mml:mi><mml:mrow	1.1	3
1361	Quantifying robustness of DFT predicted pathways and activity determining elementary steps for electrochemical reactions. Journal of Chemical Physics, 2019, 150, 041717.	1.2	14

#	Article	IF	Citations
1362	Electronic Origin of Oxygen Transport Behavior in La-Based Perovskites: A Density Functional Theory Study. Journal of Physical Chemistry C, 2019, 123, 275-290.	1.5	25
1363	Fifty Shades of Water: Benchmarking DFT Functionals against Experimental Data for Ionic Crystalline Hydrates. Journal of Chemical Theory and Computation, 2019, 15, 584-594.	2.3	12
1364	Adsorption of CO2 on biphasic and amorphous calcium phosphates: An experimental and theoretical analysis. Chemical Physics Letters, 2019, 714, 143-148.	1.2	12
1365	Push it to the limit: comparing periodic and local approaches to density functional theory for intermolecular interactions. Molecular Physics, 2019, 117, 1298-1305.	0.8	6
1366	Site-dependence of relationships between photoluminescence and applied electric field in monolayer and bilayer molybdenum disulfide. Japanese Journal of Applied Physics, 2019, 58, 015001.	0.8	1
1367	Synergistic icephobic behaviour of swollen nitrile butadiene rubber graphene and/or carbon nanotube composites. Composites Part B: Engineering, 2019, 166, 352-360.	5.9	14
1368	Recent advances on first-principles modeling for the design of materials in CO2 capture technologies. Chinese Journal of Chemical Engineering, 2019, 27, 1554-1565.	1.7	36
1369	Evaluation of methods for obtaining dispersion energies used in density functional calculations of intermolecular interactions. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	18
1370	Hybrids made of defective nanodiamonds interacting with DNA nucleobases. Nanotechnology, 2019, 30, 065601.	1.3	1
1371	Reactive and Nonreactive Scattering of HCl from Au(111): An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry C, 2019, 123, 2287-2299.	1.5	30
1372	Structures, Electronic States, and Reactions at Interfaces between LiNi_{0.5}Mn_{1.5}O₄ Cathode and Ethylene Carbonate Electrolyte: A First-Principles Study. Journal of Physical Chemistry C, 2019, 123, 2267-2277.	1.5	28
1373	Transferability of the Specific Reaction Parameter Density Functional for H2 + Pt(111) to H2 + Pt(211). Journal of Physical Chemistry C, 2019, 123, 2973-2986.	1.5	18
1374	A comparative study of mechanisms of the adsorption of CO₂ confined within grapheneâ€“MoS₂ nanosheets: a DFT trend study. Nanoscale Advances, 2019, 1, 1442-1451.	2.2	22
1375	Performance of van der Waals DFT approaches for helium diffraction on metal surfaces. Journal of Physics Condensed Matter, 2019, 31, 135901.	0.7	4
1376	A new carbon phase with direct bandgap and high carrier mobility as electron transport material for perovskite solar cells. Npj Computational Materials, 2019, 5, .	3.5	67
1377	Computational Approach to Molecular Catalysis by 3d Transition Metals: Challenges and Opportunities. Chemical Reviews, 2019, 119, 2453-2523.	23.0	260
1378	Subatomic-scale resolution with SPM: Co adatom on p(2 Ã— 1)Cu(110):O. Nanotechnology, 2019, 30, 095703.	1.3	2
1379	Metal functionalized inorganic nano-sheets as promising materials for clean energy storage. Applied Surface Science, 2019, 471, 887-892.	3.1	39

#	Article	IF	Citations
1380	Pmma-XO (X = C, Si, Ge) monolayer as promising anchoring materials for lithiumâ€“sulfur battery: a first-principles study. Nanotechnology, 2019, 30, 085405.	1.3	8
1381	Density functional theory. , 2019, , 119-159.		7
1382	Ab initio simulations of liquid electrolytes for energy conversion and storage. International Journal of Quantum Chemistry, 2019, 119, e25795.	1.0	14
1383	Hexagonal boron phosphide as a potential anode nominee for alkali-based batteries: A multi-flavor DFT study. Applied Surface Science, 2019, 471, 134-141.	3.1	49
1384	Enhanced magnetism in the VLi8 magnetic superatom supported on graphene. Applied Surface Science, 2019, 465, 207-211.	3.1	8
1385	Developments in the Atomistic Modelling of Catalytic Processes for the Production of Platform Chemicals from Biomass. ChemCatChem, 2019, 11, 357-367.	1.8	3
1386	Surface modification vs sorption strength: Study of nedaplatin drug supported on silica. Applied Surface Science, 2019, 465, 693-699.	3.1	7
1387	Firstâ€“principles study of potassium adsorption and diffusion on graphene. Molecular Physics, 2020, 118, e1581291.	0.8	14
1388	Simulations of volumetric hydrogen storage capacities of nanoporous carbons: Effect of dispersion interactions as a function of pressure, temperature and pore width. International Journal of Hydrogen Energy, 2020, 45, 5697-5709.	3.8	10
1389	Low-temperature monoclinic layer stacking in atomically thin CrI₃ crystals. 2D Materials, 2020, 7, 015007.	2.0	65
1390	Ab initio modeling and design of vanadia-based electrode materials for post-lithium batteries. Journal Physics D: Applied Physics, 2020, 53, 083001.	1.3	9
1391	Elastic properties of the molecular crystals of hydrocarbons from first principles calculations. Journal of Physics Condensed Matter, 2020, 32, 085704.	0.7	3
1392	From van der Waals interactions to structures and properties of 3,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e5014" altimg="si4.svg"><mml:msup><mml:mrow><mml:mn>3</mml:mn></mml:mrow><mml:mrow><mml:mo>â€²</mml:mo></mml:mrow><mml:mrow><mml:mo>â€²</mml:mo></mml:mrow></mml:msup></mml:math>,5,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e5024" altimg="si5.svg"><mml:msup><mml:mrow><mml:mn>5</mml:mn></mml:mrow><mml:mrow><mml:mo>â€²</mml:mo></mml:mrow><mml:mrow><mml:mo>â€²</mml:mo></mml:mrow></mml:msup></mml:math>-tetrahydrodipyrrin-1-one. Materials Chemistry and Physics, 2020, 240, 122175.	2.0	13
1393	Formaldehyde adsorption on a hydrogenated gallium nitride monolayer: A density functional theory study. Applied Surface Science, 2020, 506, 144944.	3.1	13
1394	uMBD: A Materials-Ready Dispersion Correction That Uniformly Treats Metallic, Ionic, and van der Waals Bonding. Journal of the American Chemical Society, 2020, 142, 2346-2354.	6.6	29
1395	Self-Assembly of a Two-Dimensional Sheet with Ta@Si₁₆ Superatoms and Its Magnetic and Photocatalytic Properties. Journal of Physical Chemistry C, 2020, 124, 6861-6870.	1.5	18
1396	Role of van der Waals interaction in enhancing the photon absorption capability of the MoS₂/2D heterostructure. Physical Chemistry Chemical Physics, 2020, 22, 2775-2782.	1.3	5
1397	Local dimerization and dedimerization of C60 molecules under a tip of scanning tunneling microscope: A first-principles study. Carbon, 2020, 159, 638-647.	5.4	4

#	Article	IF	Citations
1398	Electronic Polarizability as the Fundamental Variable in the Dielectric Properties of Two-Dimensional Materials. Nano Letters, 2020, 20, 841-851.	4.5	70
1399	Selective Synthesis of a Salt and a Cocrystal of the Ethionamideâ€“Salicylic Acid System. Crystal Growth and Design, 2020, 20, 906-915.	1.4	49
1400	Quasi-bonding driven abnormal isotropic thermal transport in intrinsically anisotropic nanostructure: a case of study of a phosphorus nanotube array. Nanotechnology, 2020, 31, 095704.	1.3	3
1401	Random Phase Approximation Applied to Many-Body Noncovalent Systems. Journal of Chemical Theory and Computation, 2020, 16, 427-442.	2.3	12
1402	Nâ€Doped Graphene Supported on Metalâ€Iron Carbide as a Catalyst for the Oxygen Reduction Reaction: Density Functional Theory Study. ChemSusChem, 2020, 13, 996-1005.	3.6	21
1403	Energetics and Structure of Domain Wall Networks in Minimally Twisted Bilayer Graphene under Strain. Journal of Physical Chemistry C, 2020, 124, 2120-2130.	1.5	10
1404	Understanding the Separation Mechanism of C2H6/C2H4 on Zeolitic Imidazolate Framework ZIF-7 by Periodic DFT Investigations. Journal of Physical Chemistry C, 2020, 124, 256-266.	1.5	9
1405	Hydroxyl-Assisted Phosphorene Stabilization with Robust Device Performances. Nano Letters, 2020, 20, 81-87.	4.5	21
1406	Analysis of Density-Functional Errors for Noncovalent Interactions between Charged Molecules. Journal of Physical Chemistry A, 2020, 124, 353-361.	1.1	5
1407	Structural and electronic properties of Stanene-BeO heterobilayer. Materials Research Express, 2020, 7, 015029.	0.8	6
1408	Tunable high workfunction contacts: Doped graphene. Applied Surface Science, 2020, 509, 144893.	3.1	10
1409	Oxidation-driven formation of precisely ordered antimonene nanoribbons. Journal of Physics Condensed Matter, 2020, 32, 165302.	0.7	1
1410	Poly-p-phenylenes as Novel Bulk-type Anode Materials for Potassium-Ion Batteries: A First-Principles Study. Journal of Physical Chemistry C, 2020, 124, 23045-23051.	1.5	6
1411	Semifluorinated, kinked polyarylenesviadirect arylation polycondensation. Polymer Chemistry, 2020, 11, 6928-6934.	1.9	5
1412	Improved Adsorption and Migration of Divalent Ions Over C4N Nanosheets: Potential Anode for Divalent Batteries. Surfaces and Interfaces, 2020, 21, 100758.	1.5	5
1413	A Comprehensive Study of the Bridge Site and Substrate Relaxation Asymmetry for Methanethiol Adsorption on Au(111) at Low Coverage. ACS Omega, 2020, 5, 20874-20881.	1.6	2
1414	A first-principles analysis of the charge transfer in magnesium corrosion. Scientific Reports, 2020, 10, 15006.	1.6	37
1415	A Gd@C82 single-molecule electret. Nature Nanotechnology, 2020, 15, 1019-1024.	15.6	70

#	Article	IF	Citations
1416	Two-dimensional ferromagnetic semiconductor VBr₃ with tunable anisotropy. Journal of Materials Chemistry C, 2020, 8, 14782-14788.	2.7	16
1417	Theoretical and Experimental Overview of Structural, Dielectric, Crystallographic, Electronic, Optical, and Physical Tensors of Î±-DIPAB and Iodine-Doped Î±-DIPAB Molecular Ferroelectric Crystals. Journal of Electronic Materials, 2020, 49, 7112-7132.	1.0	0
1418	Interlayer interaction controlling the properties of AB- and AA-stacked bilayer graphene-like BC14n and si2c14. Surfaces and Interfaces, 2020, 21, 100740.	1.5	12
1419	Can Single Metal Atoms Trapped in Defective h-BN/Cu(111) Improve Electrocatalysis of the H₂ Evolution Reaction?. Journal of Physical Chemistry C, 2020, 124, 23690-23698.	1.5	6
1420	Packing SierpiÅ„ski Triangles into Two-Dimensional Crystals. Journal of the American Chemical Society, 2020, 142, 17928-17932.	6.6	25
1421	Surface effects on temperature-driven spin crossover in Fe(phen)2(NCS)2. Journal of Chemical Physics, 2020, 153, 134704.	1.2	11
1422	Theoretical investigation of amino-acid adsorption on hydroxylated quartz surfaces: dispersion can determine enantioselectivity. Physical Chemistry Chemical Physics, 2020, 22, 16571-16578.	1.3	7
1423	Influence of cyano substituents on the electron density and catalytic activity towards the oxygen reduction reaction for iron phthalocyanine. The case for Fe(II) 2,3,9,10,16,17,23,24-octa(cyano)phthalocyanine. Electrochemistry Communications, 2020, 118, 106784.	2.3	20
1424	Mechanical, thermal and thermoelectric properties of MX2 (Mâ€¯=â€¯Zr, Hf; Xâ€¯=â€¯S, Se). Materials Today Communications, 2020, 25, 101434.	0.9	6
1425	Plasma-Made Graphene Nanostructures with Molecularly Dispersed F and Na Sites for Solar Desalination of Oil-Contaminated Seawater with Complete In-Water and In-Air Oil Rejection. ACS Applied Materials & Interfaces, 2020, 12, 38512-38521.	4.0	32
1426	Electronic Structure Modeling of Metalâ€“Organic Frameworks. Chemical Reviews, 2020, 120, 8641-8715.	23.0	149
1427	Effects of van der Waals Dispersion Interactions in Density Functional Studies of Adsorption, Catalysis, and Tribology on Metals. Journal of Physical Chemistry C, 2020, 124, 16926-16942.	1.5	19
1428	Universal description of potential energy surface of interlayer interaction in two-dimensional materials by first spatial Fourier harmonics. Physical Review B, 2020, 102, .	1.1	9
1429	Atomic scattering of H and N on W(100): Effect of lattice vibration and electronic excitations on the dynamics. Surface Science, 2020, 701, 121678.	0.8	5
1430	Anisotropic Poisson Effect and Deformationâ€Induced Fluorescence Change of Elastic 9,10â€Dibromoanthracene Single Crystals. Angewandte Chemie, 2020, 132, 16329-16335.	1.6	15
1431	Computational Screening of Atomically Thin Two-Dimensional Nanomaterial-Coated Cs₃Sb Heterostructures for High-Performance Photocathodes. Journal of Physical Chemistry C, 2020, 124, 26396-26403.	1.5	3
1432	Copper(I)-Based Flexible Organicâ€“Inorganic Coordination Polymer and Analogues: High-Power Factor Thermoelectrics. ACS Applied Materials & Interfaces, 2020, 12, 53841-53851.	4.0	14
1433	Doping-Induced Stacking Transition in Trilayer Graphene: Implications for Layer Stacking Manipulation. ACS Applied Nano Materials, 2020, 3, 11861-11868.	2.4	9

#	Article	IF	Citations
1434	Perspectives on van der Waals Density Functionals: The Case of TiS₂. Journal of Physical Chemistry A, 2020, 124, 9867-9876.	1.1	13
1435	Quasi-One-Dimensional Free-Electron-Like States Selected by Intermolecular Hydrogen Bonds at the Glycine/Cu(100) Interface*. Chinese Physics Letters, 2020, 37, 117301.	1.3	0
1436	Effect of van der Waals interactions on the adhesion strength at the interface of the hydroxyapatiteâ€“titanium biocomposite: a first-principles study. RSC Advances, 2020, 10, 37800-37805.	1.7	3
1437	Computational Studies on the Binding Preferences of Molybdenum(II) Phenanthroline Complexes with Duplex DNA. The Important Role of the Ancillary Ligands. Inorganic Chemistry, 2020, 59, 12711-12721.	1.9	15
1438	Why Do We Use the Materials and Operating Conditions We Use for Heterogeneous (Photo)Electrochemical Water Splitting?. ACS Catalysis, 2020, 10, 11177-11234.	5.5	89
1439	Intrinsic ferromagnetism in atomically thin two-dimensional organic-inorganic van der Waals crystals. Physical Review B, 2020, 102, .	1.1	4
1440	Defect topology and annihilation by cooperative movement of atoms in neutron-irradiated graphite. Physical Review B, 2020, 102, .	1.1	7
1441	Graphene Oxide-BiOCl Nanoparticle Composites as Catalysts for Oxidation of Volatile Organic Compounds in Nonthermal Plasmas. ACS Applied Nano Materials, 2020, 3, 9363-9374.	2.4	13
1442	Cooperative carbon capture and steam regeneration with tetraamine-appended metalâ€“organic frameworks. Science, 2020, 369, 392-396.	6.0	249
1443	An accurate and transferable machine learning potential for carbon. Journal of Chemical Physics, 2020, 153, 034702.	1.2	137
1444	Ammoniumâ€“Ammonia Complexes, N2H7+, in Ammonium closo-Borate Ammines: Synthesis, Structure, and Properties. Inorganic Chemistry, 2020, 59, 11449-11458.	1.9	6
1445	Reverse shape selectivity of hexane isomer in ligand inserted MOF-74. RSC Advances, 2020, 10, 22601-22605.	1.7	8
1446	Heat Capacity, Thermal Expansion Coefficient, and GrÃ¼neisen Parameter of CH₄, CO₂, and C₂H₆ Hydrates and Ice I_h via Density Functional Theory and Phonon Calculations. Crystal Growth and Design, 2020, 20, 5947-5955.	1.4	14
1447	Next-Generation Nonlocal van der Waals Density Functional. Journal of Chemical Theory and Computation, 2020, 16, 5893-5911.	2.3	57
1448	Computational investigation of two-dimensional LDHs and the modification of their electronic structure induced by defects. Applied Surface Science, 2020, 532, 147159.	3.1	8
1449	Dielectric ordering of water molecules arranged in a dipolar lattice. Nature Communications, 2020, 11, 3927.	5.8	33
1450	Computable Bulk and Interfacial Electronic Structure Features as Proxies for Dielectric Breakdown of Polymers. ACS Applied Materials & Interfaces, 2020, 12, 37182-37187.	4.0	21
1451	Mnâ€“Cu Transmetalation as a Strategy for the Assembly of Decoupled Metalâ€“Organic Networks on Sn/Cu(001) Surface Alloys. Journal of Physical Chemistry C, 2020, 124, 18993-19002.	1.5	4

#	Article	IF	Citations
1452	Ce0.5La0.5Ni9Ge4 compound: Why is cerium valence not 3+?. Chinese Journal of Physics, 2020, 67, 473-481.	2.0	0
1453	Structural Diversity and Trends in Properties of an Array of Hydrogen-Rich Ammonium Metal Borohydrides. Inorganic Chemistry, 2020, 59, 12733-12747.	1.9	16
1454	Carrier Distribution Control in van der Waals Heterostructures of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Mo</mml:mi><mml:mi mathvariant="normal">S</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mi>WS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>	1.5	9
1455	Local probe of the interlayer coupling strength of few-layers SnSe by contact-resonance atomic force microscopy. Frontiers of Physics, 2020, 15, 1.	2.4	8
1456	Gas Evolution in Li-Ion Batteries: Modeling Ethylene Carbonate Decomposition on LiCoO₂ in the Presence of Surface Magnetism. Journal of Physical Chemistry C, 2020, 124, 24097-24104.	1.5	6
1457	Xenon iron oxides predicted as potential Xe hosts in Earthâ€™s lower mantle. Nature Communications, 2020, 11, 5227.	5.8	27
1458	Structural properties and thermal stability of multi-walled black phosphorene nanotubes and their operation as temperature driven nanorotors. Nanoscale, 2020, 12, 18313-18321.	2.8	6
1459	Enhanced Thermal Conductivity in a Diamine-Appended Metalâ€“Organic Framework as a Result of Cooperative CO₂ Adsorption. ACS Applied Materials & Interfaces, 2020, 12, 44617-44621.	4.0	10
1460	Defect Dynamics in MAPbI₃ Polycrystalline Films: The Trapping Effect of Grain Boundaries. Helvetica Chimica Acta, 2020, 103, e2000110.	1.0	10
1461	Intercalation of Lithium into Graphite: Insights from First-Principles Simulations. Journal of Physical Chemistry C, 2020, 124, 21985-21992.	1.5	11
1462	Establishing the accuracy of density functional approaches for the description of noncovalent interactions in biomolecules. Physical Chemistry Chemical Physics, 2020, 22, 21685-21695.	1.3	4
1463	New possible candidate structure for phase IV of solid hydrogen. RSC Advances, 2020, 10, 26443-26450.	1.7	1
1464	Role of Capping Agents in the Synthesis of Salicylate-Capped Zinc Oxide Nanoparticles. ACS Applied Nano Materials, 2020, 3, 9951-9960.	2.4	7
1465	Band-like transporting and thermally durable V-shaped organic semiconductors with a phenyl key block. Journal of Materials Chemistry C, 2020, 8, 14172-14179.	2.7	7
1466	Efficient yet accurate dispersion-corrected semilocal exchangeâ€“correlation functionals for non-covalent interactions. Journal of Chemical Physics, 2020, 153, 084117.	1.2	10
1467	Strainâ€Sensitive Magnetization Reversal of a van der Waals Magnet. Advanced Materials, 2020, 32, e2004533.	11.1	119
1468	Understanding dense hydrogen at planetary conditions. Nature Reviews Physics, 2020, 2, 562-574.	11.9	29
1469	Simulations of X-ray absorption spectroscopy and energetic conformation of N-heterocyclic carbenes on Au(111). Physical Chemistry Chemical Physics, 2020, 22, 21504-21511.	1.3	6

#	Article	IF	Citations
1470	Unraveling the mechanisms of S-doped carbon nitride for photocatalytic oxygen reduction to H₂O₂. Physical Chemistry Chemical Physics, 2020, 22, 21099-21107.	1.3	29
1471	Cooperative Binding of 1-Phenylimidazole to Cobalt(II) Octaethylporphyrin on Graphite: A Quantitative Imaging and Computational Study at Molecular Resolution. Journal of Physical Chemistry C, 2020, 124, 18639-18649.	1.5	8
1472	A folded ice monolayer. Physical Chemistry Chemical Physics, 2020, 22, 20388-20393.	1.3	5
1473	Preferred oriented cation configurations in high pressure phases IV and V of methylammonium lead iodide perovskite. Scientific Reports, 2020, 10, 21138.	1.6	5
1474	Exploring high transition temperature topological superconductivity in (Li1â^'xCoxOH)CoSb superlattices. Physical Review B, 2020, 102, .	1.1	0
1475	Atomic Structure of Glassy GeTe₄ as a Playground to Assess the Performances of Density Functional Schemes Accounting for Dispersion Forces. Journal of Physical Chemistry B, 2020, 124, 11273-11279.	1.2	7
1476	Structures, electronic properties, and superconductivities of alkaline-earth metal-doped phenanthrene and charge transfer characteristics of metal-doped phenanthrene. Physical Chemistry Chemical Physics, 2020, 22, 23847-23855.	1.3	2
1477	Deep Mining Stable and Nontoxic Hybrid Organicâ€"Inorganic Perovskites for Photovoltaics via Progressive Machine Learning. ACS Applied Materials & Interfaces, 2020, 12, 57821-57831.	4.0	20
1478	Electronic energy gap closure and metal-insulator transition in dense liquid hydrogen. Physical Review B, 2020, 102, .	1.1	13
1479	Microscopic Mechanism of Van der Waals Heteroepitaxy in the Formation of MoS2/hBN Vertical Heterostructures. ACS Omega, 2020, 5, 31692-31699.	1.6	5
1480	Electronic structure, magnetism, and high-temperature superconductivity in multilayer octagraphene and octagraphite. Physical Review B, 2020, 102, .	1.1	10
1481	Lithium and Sodium Adsorption on Monolayer Tellurene. Journal of Physical Chemistry C, 2020, 124, 28074-28082.	1.5	4
1482	Robust, high-performance n-type organic semiconductors. Science Advances, 2020, 6, eaaz0632.	4.7	135
1483	Mechanical and electronic properties of van der Waals layered hcp PdH2. Scientific Reports, 2020, 10, 8037.	1.6	3
1484	Density functionals combined with van der Waals corrections for graphene adsorbed on layered materials. Physical Review B, 2020, 101, .	1.1	8
1485	Influence of interlayer stacking arrangements on carrier accumulation in bilayer graphene field effect transistors. Applied Physics Express, 2020, 13, 065006.	1.1	6
1486	In situ multimodal imaging for nanoscale visualization of tribofilm formation. Journal of Applied Physics, 2020, 127, 154303.	1.1	4
1487	The <scp>ONETEP</scp> linear-scaling density functional theory program. Journal of Chemical Physics, 2020, 152, 174111.	1.2	94

#	Article	IF	Citations
1488	Ammine Lanthanum and Cerium Borohydrides, M(BH₄)₃Â·nNH₃; Trends in Synthesis, Structures, and Thermal Properties. Inorganic Chemistry, 2020, 59, 7768-7778.	1.9	19
1489	Computational Design of a Photoresponsive Metalâ€“Organic Framework for Post Combustion Carbon Capture. Journal of Physical Chemistry C, 2020, 124, 13162-13167.	1.5	18
1490	Anisotropic Poisson Effect and Deformationâ€Induced Fluorescence Change of Elastic 9,10â€Dibromoanthracene Single Crystals. Angewandte Chemie - International Edition, 2020, 59, 16195-16201.	7.2	75
1491	Unusual Lattice Dynamics and Anisotropic Thermal Conductivity in In2Te5 Due to a Layered Structure and Planar-Coordinated Te-Chains. Chemistry of Materials, 2020, 32, 5335-5342.	3.2	22
1492	Mechanistic and microkinetic study of non-oxidative methane coupling on a single-atom iron catalyst. Communications Chemistry, 2020, 3, .	2.0	32
1493	Inclusion of Van der Waals Interactions in DFT using Wannier Functions without empirical parameters. EPJ Web of Conferences, 2020, 230, 00010.	0.1	1
1494	Mechanism of the Accelerated Water Formation Reaction under Interfacial Confinement. ACS Catalysis, 2020, 10, 6119-6128.	5.5	20
1495	Hexagonal layered group IVâ€“VI semiconductors and derivatives: fresh blood of the 2D family. Nanoscale, 2020, 12, 13450-13459.	2.8	20
1496	XO-PBC: An Accurate and Efficient Method for Molecular Crystals. Journal of Chemical Theory and Computation, 2020, 16, 4271-4285.	2.3	10
1497	Application of the training of density functional theory potentials within machine learning to adsorptions and reactionÂpaths on Platinum surfaces. Materials Chemistry and Physics, 2020, 253, 123407.	2.0	5
1498	Gap variability upon packing in organic photovoltaics. PLoS ONE, 2020, 15, e0234115.	1.1	0
1499	Valley polarization investigation of GeS under high pressure. Physical Review B, 2020, 101, .	1.1	10
1500	Origin of ferromagnetism and the effect of doping on Fe₃GeTe₂. Nanoscale, 2020, 12, 13501-13506.	2.8	41
1501	Long structures of H2O molecules adsorbed on the V2O5(0 0 1) surface. A DFTÂ+ÂU study including van der Waals interactions. Chemical Physics Letters, 2020, 749, 137408.	1.2	0
1502	Hydrogen-Bonded Small-Molecular Crystals Yielding Strong Ferroelectric and Antiferroelectric Polarizations. Journal of the Physical Society of Japan, 2020, 89, 051009.	0.7	51
1503	Phonons and Anomalous Lattice Behavior in KMnAg₃(CN)₆ and KNiAu₃(CN)₆: Inelastic Neutron Scattering and First-Principles Calculations. Journal of Physical Chemistry C, 2020, 124, 7216-7228.	1.5	2
1504	Energy Gap Closure of Crystalline Molecular Hydrogen with Pressure. Physical Review Letters, 2020, 124, 116401.	2.9	24
1505	[n]Phenacenes: Promising Organic Anodes for Potassium-Ion Batteries. Journal of Physical Chemistry C, 2020, 124, 6964-6970.	1.5	13

#	Article	IF	Citations
1506	Exfoliation of zirconium aminophosphonates: investigation into their electronic structures by ab initio calculations. New Journal of Chemistry, 2020, 44, 10111-10118.	1.4	5
1507	Noncovalent Quantum Machine Learning Corrections to Density Functionals. Journal of Chemical Theory and Computation, 2020, 16, 2647-2653.	2.3	18
1508	Divergent Adsorption-Dependent Luminescence of Amino-Functionalized Lanthanide Metalâ€“Organic Frameworks for Highly Sensitive NO₂ Sensors. Journal of Physical Chemistry Letters, 2020, 11, 3362-3368.	2.1	50
1509	Extension and evaluation of the D4 London-dispersion model for periodic systems. Physical Chemistry Chemical Physics, 2020, 22, 8499-8512.	1.3	138
1510	Excellent thermoelectric performance induced by interface effect in MoS₂/MoSe₂ van der Waals heterostructure. Journal of Physics Condensed Matter, 2020, 32, 055302.	0.7	43
1511	Emergent superconductivity in two-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>NiTe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> crystals. Physical Review B, 2020, 101, .	1.1	83
1512	Coordinatively unsaturated metal sites (open metal sites) in metalâ€“organic frameworks: design and applications. Chemical Society Reviews, 2020, 49, 2751-2798.	18.7	449
1513	Octopus, a computational framework for exploring light-driven phenomena and quantum dynamics in extended and finite systems. Journal of Chemical Physics, 2020, 152, 124119.	1.2	210
1514	In Situ Assessment of Intrinsic Strength of X-Iâ‹¯OA-Type Halogen Bonds in Molecular Crystals with Periodic Local Vibrational Mode Theory. Molecules, 2020, 25, 1589.	1.7	26
1515	Sublimation Properties of Î±,Ï‰â€Diamines Revisited from Firstâ€Principles Calculations. ChemPhysChem, 2020, 21, 1184-1194.	1.0	6
1516	Activation of topological insulator phase in kagomÃ©-type bilayers by interlayer coupling: The cases of Ni(CO)4 and Pd(CO)4. Applied Physics Letters, 2020, 116, .	1.5	3
1517	Bulk and Surface Electronic Structure of the Dual-Topology Semimetal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Pt</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow> Physical Review Letters, 2020, 124, 106402.	2.9	40
1518	Tuning the Catalytic Activity of a Quantum Nutcracker for Hydrogen Dissociation. Surfaces, 2020, 3, 40-47.	1.0	2
1519	Asymptotic Pairwise Dispersion Corrections Can Describe Layered Materials Accurately. Journal of Physical Chemistry Letters, 2020, 11, 2298-2302.	2.1	17
1520	Closing the Gap Between Experiment and Theory: Reactive Scattering of HCl from Au(111). Journal of Physical Chemistry C, 2020, 124, 15944-15960.	1.5	18
1521	Chirality-induced relaxor properties in ferroelectric polymers. Nature Materials, 2020, 19, 1169-1174.	13.3	93
1522	Metal-Free Hybrid Organicâ€“Inorganic Perovskites for Photovoltaics. Journal of Physical Chemistry Letters, 2020, 11, 5938-5947.	2.1	12
1523	Trends and Outlook of Computational Chemistry and Microkinetic Modeling for Catalytic Synthesis of Methanol and DME. Catalysts, 2020, 10, 655.	1.6	16

#	Article	IF	Citations
1524	Aldehyde trapping by self-propagating atom-exchange reactions on a gallium nitride monolayer: role of the molecule complexity. New Journal of Chemistry, 2020, 44, 12843-12849.	1.4	6
1525	Screening nature of the van der Waals density functional method: a review and analysis of the many-body physics foundation. Journal of Physics Condensed Matter, 2020, 32, 393001.	0.7	28
1526	Tuning energy barriers by doping 2D group-IV monochalcogenides. Journal of Applied Physics, 2020, 127, .	1.1	4
1527	Polymer Structure Prediction from First Principles. Journal of Physical Chemistry Letters, 2020, 11, 5823-5829.	2.1	20
1528	Superlubricity in phosphorene identified by means of ab initio calculations. 2D Materials, 2020, 7, 025033.	2.0	32
1529	Nanoscale First-Principles Electronic Structure Simulations of Materials Relevant to Organic Electronics. , 2020, , 89-131.		1
1530	Tunable spin-polarized band gap in Si₂/NiI₂ vdW heterostructure. RSC Advances, 2020, 10, 8927-8935.	1.7	6
1531	Density-functional theory prediction of the elastic constants of ice Ih. Journal of Chemical Physics, 2020, 152, 084502.	1.2	4
1532	Benchmarking PBE+D3 and SCAN+rVV10 methods using potential energy surfaces generated with MP2+Î”CCSD(T) calculation. Chinese Physics B, 2020, 29, 013102.	0.7	2
1533	Existence of untypical halogen-involving interactions in crystal packings: a statistical and first-principles study. CrystEngComm, 2020, 22, 2756-2765.	1.3	13
1534	First-principles prediction of a two-dimensional vanadium carbide (MXene) as the anode for lithium ion batteries. Physical Chemistry Chemical Physics, 2020, 22, 5807-5818.	1.3	40
1535	Chemisorption characteristics of pyridine on Rh, Pd, Pt and Ni(1â€‰1â€‰1). Electronic Structure, 2020, 2, 015001.	1.0	2
1536	A theoretical study of the influence of gold nanoplatelets sites in C C coupling reaction. Molecular Catalysis, 2020, 485, 110845.	1.0	0
1537	Fluorination of Organic Spacer Impacts on the Structural and Optical Response of 2D Perovskites. Frontiers in Chemistry, 2019, 7, 946.	1.8	14
1538	Probing structural changes upon carbon monoxide coordination to single metal adatoms. Journal of Chemical Physics, 2020, 152, 051102.	1.2	4
1539	Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics. 1. Theory, Algorithm, and Performance. Journal of Chemical Theory and Computation, 2020, 16, 3757-3785.	2.3	29
1540	Room Temperature Commensurate Charge Density Wave on Epitaxially Grown Bilayer 2H-Tantalum Sulfide on Hexagonal Boron Nitride. ACS Nano, 2020, 14, 3917-3926.	7.3	27
1541	Structural stability and optoelectronic properties of tetragonal MAPbI₃ under strain. Nanotechnology, 2020, 31, 225204.	1.3	19

#	Article	IF	Citations
1542	Long-range behavior of a nonlocal correlation-energy density functional based on the random-phase approximation. Physical Review B, 2020, 101, .	1.1	1
1543	On tuning the cytotoxicity of Ti₃C₂ (MXene) flakes to cancerous and benign cells by post-delamination surface modifications. 2D Materials, 2020, 7, 025018.	2.0	63
1544	Lead-free hybrid organic-inorganic perovskites for solar cell applications. Journal of Chemical Physics, 2020, 152, 014104.	1.2	6
1545	Modified Density Functional Dispersion Correction for Inorganic Layered MFX Compounds (M = Ca, Sr,) Tj ETQq1 1 0.784314 rgBT /O	1.1	5
1546	Physicochemical properties of l- and dl-valine: first-principles calculations. Amino Acids, 2020, 52, 425-433.	1.2	5
1547	Superior sensitivity of metal functionalized boron carbide (BC3) monolayer towards carbonaceous pollutants. Applied Surface Science, 2020, 512, 145637.	3.1	15
1548	Feâ€porphyrin on Co(001) and Cu(001): A Comparative Dispersionâ€augmented Density Functional Theory Study. Israel Journal of Chemistry, 2020, 60, 870-875.	1.0	0
1549	A Helical Monolayer Ice. Journal of Physical Chemistry Letters, 2020, 11, 3860-3865.	2.1	9
1550	Thermodynamics of the insulator-metal transition in dense liquid deuterium. Physical Review B, 2020, 101, .	1.1	6
1551	Physi-Sorption of H2 on Pure and Boronâ€“Doped Graphene Monolayers: A Dispersionâ€“Corrected DFT Study. Journal of Carbon Research, 2020, 6, 15.	1.4	13
1552	Excellent thermoelectric performance in weak-coupling molecular junctions with electrode doping and electrochemical gating. Science China: Physics, Mechanics and Astronomy, 2020, 63, 1.	2.0	51
1553	Functionalized Two-Dimensional Nanoporous Graphene as Efficient Global Anode Materials for Li-, Na-, K-, Mg-, and Ca-Ion Batteries. Journal of Physical Chemistry C, 2020, 124, 9734-9745.	1.5	28
1554	What is â€œmany-bodyâ€•dispersion and should I worry about it?. Physical Chemistry Chemical Physics, 2020, 22, 8266-8276.	1.3	30
1555	Work function and band alignment of few-layer violet phosphorene. Journal of Materials Chemistry A, 2020, 8, 8586-8592.	5.2	43
1556	Improved Predictive Tools for Structural Properties of Metalâ€“Organic Frameworks. Molecules, 2020, 25, 1552.	1.7	7
1557	Dynamics Studies of O₂ Collision on Pt(111) Using a Global Potential Energy Surface. Journal of Physical Chemistry C, 2020, 124, 10573-10583.	1.5	7
1558	Influence of Interlayer Stacking on Gate-Induced Carrier Accumulation in Bilayer MoS₂. ACS Applied Electronic Materials, 2020, 2, 1352-1357.	2.0	12
1559	Alkynyl Linkers as a Design Tool to Gain Control over the Self-Assembly of Meso-Substituted Porphyrins on HOPG. Langmuir, 2020, 36, 4897-4907.	1.6	4

#	Article	IF	Citations
1560	Identification of active sites for CO₂ hydrogenation in Fe catalysts by first-principles microkinetic modelling. Journal of Materials Chemistry A, 2020, 8, 13014-13023.	5.2	30
1561	Plastic and Superionic Helium Ammonia Compounds under High Pressure and High Temperature. Physical Review X, 2020, 10, .	2.8	28
1562	Anisotropic 2D excitons unveiled in organicâ€“inorganic quantum wells. Materials Horizons, 2021, 8, 197-208.	6.4	17
1563	Hexagonal boron phosphide monolayer exfoliation induced by arsenic incorporation in the BP (1 1 1) surface: A DFT study. Applied Surface Science, 2021, 538, 148163.	3.1	8
1564	Exotic Structural and Optoelectronic Properties of Layered Halide Double Perovskite Polymorphs. Advanced Functional Materials, 2021, 31, 2008620.	7.8	5
1565	Mechanism of formaldehyde and formic acid formation on (101)-TiO₂@Cu₄ systems through CO₂ hydrogenation. Sustainable Energy and Fuels, 2021, 5, 564-574.	2.5	4
1566	Understanding the Selectivity of the Oxygen Reduction Reaction at the Atomistic Level on Nitrogenâ€Doped Graphitic Carbon Materials. Advanced Energy Materials, 2021, 11, 2002459.	10.2	63
1567	Designing new SRP density functionals including non-local vdW-DF2 correlation for H2 + Cu(111) and their transferability to H2 + Ag(111), Au(111) and Pt(111). Physical Chemistry Chemical Physics, 2021, 23, 7875-7901.	1.3	9
1568	Computational Methods in Heterogeneous Catalysis. Chemical Reviews, 2021, 121, 1007-1048.	23.0	198
1569	Study of the Elastic Properties of the Energetic Molecular Crystals Using Density Functionals with van der Waals Corrections. ACS Omega, 2021, 6, 642-648.	1.6	11
1570	First-Principles Insights into Plasmon-Induced Catalysis. Annual Review of Physical Chemistry, 2021, 72, 99-119.	4.8	41
1571	Microwave-Assisted Synthesis, Characterization and Modeling of CPO-27-Mg Metal-Organic Framework for Drug Delivery. Molecules, 2021, 26, 426.	1.7	4
1572	Benchmarking London dispersion corrected density functional theory for noncovalent ionâ€“Ï€ interactions. Physical Chemistry Chemical Physics, 2021, 23, 11635-11648.	1.3	31
1573	Tunable Interface of Ruthenium Porphyrins and Silver. Journal of Physical Chemistry C, 2021, 125, 3215-3224.	1.5	14
1574	Ab Initio Study of Adsorption of Fission Gas Atoms Xe and Kr on MoS₂ Monolayer Functionalized with 3d Transition Metals. Journal of Physical Chemistry C, 2021, 125, 1493-1508.	1.5	14
1575	First principles modeling of polymer encapsulant degradation in Si photovoltaic modules. Physical Chemistry Chemical Physics, 2021, 23, 10357-10364.	1.3	2
1576	Metastable piezoelectric group-IV monochalcogenide monolayers with a buckled honeycomb structure. Physical Review B, 2021, 103, .	1.1	23
1577	Ultra-low thermal conductivity and high thermoelectric performance of monolayer BiP₃: a first principles study. Physical Chemistry Chemical Physics, 2021, 23, 19834-19840.	1.3	2

#	Article	IF	Citations
1578	Multi-phonon proton transfer pathway in a molecular organic ferroelectric crystal. Physical Chemistry Chemical Physics, 2021, 23, 2885-2890.	1.3	3
1579	Structural and electronic properties of layered nanoporous organic nanocrystals. RSC Advances, 2021, 11, 5773-5784.	1.7	4
1580	Revised local atomic potential method for predicting properties of energetic materials. Journal of Energetic Materials, 0, , 1-17.	1.0	0
1581	The discovery of conductive ionic bonds in NiO/Ni transparent counter electrodes for electrochromic smart windows with an ultra-long cycling life. Materials Advances, 0, , .	2.6	13
1582	Tailoring the magnetic ordering of the Cr₄O₅/Fe(001) surface via a controlled adsorption of C₆₀ organic molecules. Physical Chemistry Chemical Physics, 2021, 23, 7948-7954.	1.3	1
1583	Unravelling the K-promotion effect in highly active and stable Fe5C2 nanoparticles for catalytic linear Î±-olefin production. Materials Advances, 2021, 2, 1050-1058.	2.6	3
1584	Polycrystalline Few-Layer Graphene as a Durable Anticorrosion Film for Copper. Nano Letters, 2021, 21, 1161-1168.	4.5	39
1585	Syngas molecules as probes for defects in 2D hexagonal boron nitride: their adsorption and vibrations. Physical Chemistry Chemical Physics, 2021, 23, 7988-8001.	1.3	9
1586	Computational approaches to dissociative chemisorption on metals: towards chemical accuracy. Physical Chemistry Chemical Physics, 2021, 23, 8962-9048.	1.3	47
1587	Electrically tunable band gap in strained h-BN/silicene van der Waals heterostructures. Physical Chemistry Chemical Physics, 2021, 23, 17033-17040.	1.3	4
1588	Significantly enhanced thermoelectric performance in intermediate weak-coupling C₈-BTBT molecular junctions with p/n-type electrode doping. Journal of Materials Chemistry C, 2021, 9, 12322-12329.	2.7	8
1589	Electrostatic patterning on graphene with dipolar self-assembly. Physical Chemistry Chemical Physics, 2021, 23, 22014-22021.	1.3	5
1590	Tetrazine molecules as an efficient electronic diversion channel in 2D organicâ€“inorganic perovskites. Materials Horizons, 2021, 8, 1547-1560.	6.4	24
1591	Ultrafast charge dynamics and photoluminescence in bilayer MoS₂. 2D Materials, 2021, 8, 025018.	2.0	7
1592	A revised mechanism of band gap evolution of TMDC nanotubes and its application to Janus TMDC nanotubes: negative electron and hole compressibility. Journal of Materials Chemistry C, 0, , .	2.7	7
1593	Decoupled strain response of ferroic properties in a multiferroic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">VOCl</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> monolayer. Physical Review B, 2021, 103, .	1.1	9
1594	Structural and electronic properties of solid molecular hydrogen from many-electron theories. Physical Review B, 2021, 103, .	1.1	3
1595	Atomically Alloyed Feâ€“Co Catalyst Derived from a N-Coordinated Co Single-Atom Structure for CO₂ Hydrogenation. ACS Catalysis, 2021, 11, 2267-2278.	5.5	48

#	Article	IF	Citations
1596	Photocatalytic Câ€“C Coupling from Carbon Dioxide Reduction on Copper Oxide with Mixed-Valence Copper(I)/Copper(II). Journal of the American Chemical Society, 2021, 143, 2984-2993.	6.6	206
1597	First-principles study of an <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>S</mml:mi><mml:mo>=</mml:mo><mml:mn>1</mml:mn></mml:mrow></mml:math> quasi one-dimensional quantum molecular magnetic material. Physical Review B, 2021, 103, .	1.1	1
1598	High-throughput bandstructure simulations of van der Waals hetero-bilayers formed by 1T and 2H monolayers. Npj 2D Materials and Applications, 2021, 5, .	3.9	18
1599	Development of a Multiphase Beryllium Equation of State and Physics-based Variations. Journal of Physical Chemistry A, 2021, 125, 1610-1636.	1.1	16
1600	Millisecond lattice gasification for high-density CO ₂ - and O ₂ -sieving nanopores in single-layer graphene. Science Advances, 2021, 7, .	4.7	47
1601	First-Principles Calculations on Thermoelectric Properties of Layered Transition Metal Phosphides MP2 (M = Ni, Pd, Pt). Journal of Electronic Materials, 2021, 50, 2510-2520.	1.0	6
1602	Carrier distribution control in bilayer graphene under a perpendicular electric field by interlayer stacking arrangements. Applied Physics Express, 2021, 14, 035001.	1.1	4
1603	Mechanically Enhanced Catalytic Reduction of Carbon Dioxide over Defect Hexagonal Boron Nitride. ACS Sustainable Chemistry and Engineering, 2021, 9, 2447-2455.	3.2	25
1604	Quantify point defects in monolayer tungsten diselenide. Nanotechnology, 2021, 32, 255701.	1.3	6
1605	Describing adsorption of benzene, thiophene, and xenon on coinage metals by using the Zarembaâ€“Kohn theory-based model. Journal of Chemical Physics, 2021, 154, 124705.	1.2	4
1606	Electronic and Magnetic Diversity of Graphone/Graphene Superlattices. Chemistry of Materials, 2021, 33, 2090-2098.	3.2	5
1607	Van der Waals epitaxial growth of air-stable CrSe2 nanosheets with thickness-tunable magnetic order. Nature Materials, 2021, 20, 818-825.	13.3	206
1608	Assembly and Manipulation of a Prototypical N-Heterocyclic Carbene with a Metalloporphyrin Pedestal on a Solid Surface. Journal of the American Chemical Society, 2021, 143, 4433-4439.	6.6	18
1609	Dielectric continuum methods for quantum chemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1519.	6.2	91
1610	Interfacial Enhancement of Photovoltaic Performance in MAPbI₃/CsPbI₃ Superlattice. ACS Applied Materials & Interfaces, 2021, 13, 14679-14687.	4.0	13
1611	On-surface preparation of coordinated lanthanide-transition-metal clusters. Nature Communications, 2021, 12, 1619.	5.8	20
1612	Carrier Redistribution in van der Waals Nanostructures Consisting of Bilayer Graphene and Buckybowl: Implications for Piezoelectric Devices. ACS Applied Nano Materials, 2021, 4, 3007-3012.	2.4	4
1613	Multilevel screening of computationâ€ready, experimental metalâ€organic frameworks for natural gas purification. AICHE Journal, 2021, 67, e17279.	1.8	6

#	Article	IF	Citations
1614	Performance of Made Simple Meta-GGA Functionals with rVV10 Nonlocal Correlation for H₂ + Cu(111), D₂ + Ag(111), H₂ + Au(111), and D₂ + Pt(111). Journal of Physical Chemistry C, 2021, 125, 8993-9010.	1.5	11
1615	Dataset of noncovalent intermolecular interaction energy curves for 24 small high-spin open-shell dimers. Journal of Chemical Physics, 2021, 154, 134106.	1.2	5
1616	A Good Prediction of the Overall Reaction Rate May Not Mean a Correct Description of the Reaction Kinetics: A Case Study for CO Oxidation on RuO₂(110) Surfaces. Journal of Physical Chemistry C, 2021, 125, 9169-9177.	1.5	7
1617	Metal-semiconductor transition in the supercooled liquid phase of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ge</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> and GeTe compounds. Physical Review Materials, 2021, 5, .	3.1	11
1618	Methanol carbonylation over acid mordenite: Insights from ab initio molecular dynamics and machine learning thermodynamic perturbation theory. Journal of Catalysis, 2021, 396, 166-178.	3.1	11
1619	Novel high voltage polymer insulators using computational and data-driven techniques. Journal of Chemical Physics, 2021, 154, 174906.	1.2	12
1620	Uncertainty of exchangeâ€correlation functionals in density functional theory calculations for lithiumâ€based solid electrolytes on the case study of lithium phosphorus oxynitride. Journal of Computational Chemistry, 2021, 42, 1283-1295.	1.5	6
1621	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg"><mml:msub><mml:mrow		

#	Article	IF	Citations
1632	Quasiperiodic modulation of electronic states at edges of tellurium nanoribbons on <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>graphene</mml:mi><mml:mo>/</mml:mo><mml:mn>6</mml:mn><mml:mn><mr Physical Review B, 2021, 103, .	1.1	3
1633	Interferometric 4Dâ€STEM for Lattice Distortion and Interlayer Spacing Measurements of Bilayer and Trilayer 2D Materials. Small, 2021, 17, e2100388.	5.2	13
1635	Phase Diagrams for sII Clathrate Hydrates of CO2 from First-Principles Thermodynamics. Journal of Physical Chemistry A, 2021, 125, 5956-5962.	1.1	1
1636	Band alignment and interlayer hybridization in monolayer organic/WSe2 heterojunction. Nano Research, 0, , 1.	5.8	10
1637	Complete Reaction Cycle for Methane-to-Methanol Conversion over Cu-SSZ-13: First-Principles Calculations and Microkinetic Modeling. Journal of Physical Chemistry C, 2021, 125, 14681-14688.	1.5	10
1638	CONI-Net: Machine Learning of Separable Intermolecular Force Fields. Journal of Chemical Theory and Computation, 2021, 17, 4996-5006.	2.3	5
1639	Prediction of a stable helium-hydrogen compound: First-principles simulations. Physical Review B, 2021, 104, .	1.1	4
1640	Effects of Charge Transfer on the Critical Distance of the Interlayer Ferromagnetic Order Transition in SCrSeâ€Based van der Waals Bilayers. Physica Status Solidi - Rapid Research Letters, 2021, 15, 2100213.	1.2	0
1641	Revised Huang-Carter nonlocal kinetic energy functional for semiconductors and their surfaces. Physical Review B, 2021, 104, .	1.1	15
1642	Formation of porous ice frameworks at room temperature. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	7
1643	Emergence of Nontrivial Spin Textures in Frustrated Van Der Waals Ferromagnets. Nanomaterials, 2021, 11, 1770.	1.9	9
1644	Future directions of chemical theory and computation. Pure and Applied Chemistry, 2021, 93, 1423-1433.	0.9	3
1645	Influence of Defects and Linker Exchange on Removal of Phosphate Using MOFs with the Node Structure M₆(OH)₄(O)₄ for M = Hf, Zr, or Ce. Chemistry of Materials, 2021, 33, 5730-5737.	3.2	10
1646	Experimental Adhesion Energy in van der Waals Crystals and Heterostructures from Atomically Thin Bubbles. Physical Review Letters, 2021, 127, 046101.	2.9	36
1647	Theory-Guided Discovery of Novel Materials. Journal of Physical Chemistry Letters, 2021, 12, 6499-6513.	2.1	11
1648	Graphene-hexagonal boron nitride van der Waals heterostructures: an examination of the effects of different van der Waals corrections. Materials Research Express, 2021, 8, 085601.	0.8	12
1649	Density Functional Theory for Electrocatalysis. Energy and Environmental Materials, 2022, 5, 157-185.	7.3	95
1650	Enhanced H₂ Storage Capacity of Bilayer Hexagonal Boron Nitride (h-BN) Incorporating van der Waals Interaction under an Applied External Electric Field. ACS Omega, 2021, 6, 22374-22382.	1.6	17

#	Article	IF	Citations
1651	Rangeâ€separated multiconfigurational density functional theory methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 0, , e1566.	6.2	9
1652	Pressure-induced structural and electronic transitions in InTeI. Physical Review B, 2021, 104, .	1.1	3
1653	Layered Double Hydroxide-Derived Intermetallic Ni₃GaC_{0.25} Catalysts for Dry Reforming of Methane. ACS Catalysis, 2021, 11, 11091-11102.	5.5	26
1654	Rational Design of Highly Stable and Active MXeneâ€Based Bifunctional ORR/OER Doubleâ€Atom Catalysts. Advanced Materials, 2021, 33, e2102595.	11.1	137
1655	Engineering Na+-layer spacings to stabilize Mn-based layered cathodes for sodium-ion batteries. Nature Communications, 2021, 12, 4903.	5.8	109
1656	Gas Transport across Carbon Nitride Nanopores: A Comparison of van der Waals Functionals against the Random-Phase Approximation. Journal of Physical Chemistry C, 2021, 125, 18896-18904.	1.5	4
1657	Gate Control of Spin-Layer-Locking FETs and Application to Monolayer LuIO. Nano Letters, 2021, 21, 7631-7636.	4.5	2
1658	Toward the Proper Selection of Carbon Electrode Materials for Energy Storage Applications: Experimental and Theoretical Insights. Energy & Fuels, 2021, 35, 13426-13437.	2.5	12
1659	New Insights on the Interaction of Phenanthroline Based Ligands and Metal Complexes and Polyoxometalates with Duplex DNA and G-Quadruplexes. Molecules, 2021, 26, 4737.	1.7	21
1660	Phase transition mechanism of hexagonal graphite to hexagonal and cubic diamond: ab initio simulation. Journal of Physics Condensed Matter, 2021, 33, 425403.	0.7	1
1661	Study of the molybdenum dichalcogenide crystals: recent developments and novelty of the P-MoS2 structure. Journal of Molecular Modeling, 2021, 27, 268.	0.8	5
1662	Cross-plane thermal transport in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></ Physical Review B, 2021, 104, .	1.1	4
1663	Reduced-gradient analysis of van der Waals complexes. Electronic Structure, 2021, 3, 034009.	1.0	7
1664	Tuning Surface States of Metal/Polymer Contacts Toward Highly Insulating Polymer-Based Dielectrics. ACS Applied Materials & Interfaces, 2021, 13, 46142-46150.	4.0	31
1665	A DFT study on AlN nanotubes and nanosheets as anodes for Mg-ion batteries. Computational and Theoretical Chemistry, 2021, 1203, 113352.	1.1	2
1666	Importance of Van der Waals Interactions in Hydrogen Adsorption on a Silicon-carbide Nanotube Revisited with vdW-DFT and Quantum Monte Carlo. ACS Omega, 2021, 6, 24630-24636.	1.6	12
1667	vdW-DF-ahcx: a range-separated van der Waals density functional hybrid. Journal of Physics Condensed Matter, 2021, 34, .	0.7	7
1668	Vibrational Signature of Metallophilic Interactions in [Pt(terpy)Cl][Au(CN)₂]. Journal of Physical Chemistry C, 2021, 125, 22188-22194.	1.5	7

#	Article	IF	Citations
1669	Understanding Waterâ€“Zeolite Interactions: On the Accuracy of Density Functionals. Journal of Physical Chemistry C, 2021, 125, 20261-20274.	1.5	10
1670	Engineering dâ€p Orbital Hybridization in Singleâ€Atom Metalâ€Embedded Threeâ€Dimensional Electrodes for Liâ€“S Batteries. Advanced Materials, 2021, 33, e2105947.	11.1	209
1671	Interlayer Interaction Induced Layer-Dependent Catalytic Activity toward a Hydrogen Evolution Reaction on Two-Dimensional PtSe2. Journal of Physical Chemistry C, 2021, 125, 19716-19723.	1.5	1
1672	Study on the electronic properties of M6X6 (MÂ=ÂMo, W; X Â=ÂS, Se, Te) nanowire arrays. Chemical Physics Letters, 2021, 780, 138905.	1.2	0
1673	Multiscale modeling studies for exploring lignocellulosic biomass structure. , 2022, , 257-289.		2
1674	Force fields for waterâ€“surface interaction: is reproduction of the experimental water contact angle enough?. Chemical Communications, 2021, 57, 3355-3358.	2.2	3
1675	Surface self-assembly involving the interaction between S and N atoms. Chemical Communications, 2021, 57, 1328-1331.	2.2	3
1676	Morphology-induced dielectric enhancement in polymer nanocomposites. Nanoscale, 2021, 13, 10933-10942.	2.8	27
1677	Theoretical understanding of the properties of stepped iron surfaces with van der Waals interaction corrections. Physical Chemistry Chemical Physics, 2021, 23, 2649-2657.	1.3	8
1678	Pressure Induced Hydrogen Orderâ€“Disorder Transition in Î²-Ni(OH)₂. Journal of Physical Chemistry C, 2021, 125, 2785-2792.	1.5	7
1679	Suppression of dynamic disorder by electrostatic interactions in structurally close organic semiconductors. Physical Chemistry Chemical Physics, 2021, 23, 15485-15491.	1.3	10
1680	In situ TEM study of edge reconstruction and evolution in monolayer black phosphorus. Nanoscale, 2021, 13, 4133-4139.	2.8	9
1681	Adsorption of Transition Metal Catalysts on Carbon Supports: A Theoretical Perspective. Johnson Matthey Technology Review, 2022, 66, 4-20.	0.5	1
1682	Designing nanoscale capacitors based on twin-graphene. Physical Chemistry Chemical Physics, 2021, 23, 16268-16276.	1.3	16
1683	A first-principles understanding of the CO-assisted NO reduction on the IrRu/Al₂O₃catalyst under O₂-rich conditions. Catalysis Science and Technology, 2021, 11, 4353-4366.	2.1	5
1684	Architecture and Function of Biohybrid Solar Cell and Solar-to-Fuel Nanodevices. Springer Series in Materials Science, 2020, , 227-274.	0.4	2
1685	Database-Driven High-Throughput Calculations and Machine Learning Models for Materials Design. Lecture Notes in Physics, 2020, , 377-395.	0.3	12
1686	Electronic Structure of Exfoliated MoS2. Lecture Notes in Nanoscale Science and Technology, 2014, , 37-51.	0.4	4

#	Article	IF	Citations
1687	Band gap tuning in aluminum doped two-dimensional hexagonal boron nitride. Materials Chemistry and Physics, 2020, 250, 123176.	2.0	19
1688	Rechargeable Alkali-Ion Battery Materials: Theory and Computation. Chemical Reviews, 2020, 120, 6977-7019.	23.0	145
1689	CO Adsorption on Graphite-like ZnO Bilayers Supported on Cu(111), Ag(111), and Au(111) Surfaces. Journal of Physical Chemistry C, 2017, 121, 27453-27461.	1.5	34
1690	On the van der Waals Epitaxy of Homo-/Heterostructures of Transition Metal Dichalcogenides. ACS Applied Materials & Interfaces, 2020, 12, 27508-27517.	4.0	22
1691	Orderâ€“disorder phase transition induced by proton transfer in a co-crystal of 2,4-dichlorobenzoic acid and trimethylamine N-oxide. CrystEngComm, 2017, 19, 3753-3759.	1.3	3
1692	Magnetism and stability of all primitive stacking patterns in bilayer chromium trihalides. Journal Physics D: Applied Physics, 2021, 54, 064002.	1.3	13
1693	Importance of van der Waals interactions for ab initio studies of topological insulators. Journal of Physics Condensed Matter, 2021, 33, 035702.	0.7	9
1694	Tunable electronic structures of germanane/antimonene van der Waals heterostructures using an external electric field and normal strain. Chinese Physics B, 2020, 29, 076102.	0.7	8
1695	Two ultra-stable novel allotropes of tellurium few-layers*. Chinese Physics B, 2020, 29, 097103.	0.7	5
1696	2D 1Tâ€²-MoS₂-WS₂ van der Waals heterostructure for hydrogen evolution reaction: dispersion-corrected density functional theory calculations. Materials Research Express, 2020, 7, 075506.	0.8	13
1697	Bethe-Slater-curve-like behavior and interlayer spin-exchange coupling mechanisms in two-dimensional magnetic bilayers. Physical Review B, 2020, 102, .	1.1	46
1698	Temporally decoherent and spatially coherent vibrations in metal halide perovskites. Physical Review B, 2020, 102, .	1.1	7
1699	Jacutingaite-family: A class of topological materials. Physical Review B, 2020, 102, .	1.1	13
1700	Evaluation of van der Waals density functionals for layered materials. Physical Review Materials, 2018, 2, .	0.9	71
1701	Thermal expansion in dispersion-bound molecular crystals. Physical Review Materials, 2018, 2, .	0.9	18
1702	Vibrational and dielectric properties of the bulk transition metal dichalcogenides. Physical Review Materials, 2018, 2, .	0.9	25
1703	Intrinsic core level photoemission of suspended monolayer graphene. Physical Review Materials, 2018, 2, .	0.9	15
1704	Ab initioinvestigation of monoclinic phase stability and martensitic transformation in crystalline polyethylene. Physical Review Materials, 2018, 2, .	0.9	14

#	Article	IF	Citations
1705	Prediction of pressure-induced stabilization of noble-gas-atom compounds with alkali oxides and alkali sulfides. Physical Review Materials, 2019, 3, .	0.9	20
1706	Microscopic understanding of magnetic interactions in bilayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CrI</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> Physical Review Materials, 2019, 3, .	0.9	127
1707	Nonlocal van der Waals functionals for solids: Choosing an appropriate one. Physical Review Materials, 2019, 3, .	0.9	65
1708	Van der Waals forces stabilize low-energy polymorphism in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> : Implications for the crystallization anomaly. Physical Review Materials, 2019, 3, .	0.9	9
1709	Dynamics of graphene/Al interfaces using COMB3 potentials. Physical Review Materials, 2019, 3, .	0.9	7
1710	Untwinned <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>YBa</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mrow><mml:mn>7</mml:mn><mml:mo>â”</mml:mo><mml:mi>Î´</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math> thin films on MgO substrates: A platform to study strain effects on the local orders in cuprates. Physical Review Materials, 2019, 3, .	0.9	9
1711	Group-IV monochalcogenide monolayers: Two-dimensional ferroelectrics with weak intralayer bonds and a phosphorenelike monolayer dissociation energy. Physical Review Materials, 2019, 3, .	0.9	19
1712	Comprehensive analysis of the influence of dispersion on group-14 rutile-type solids. Physical Review Materials, 2020, 4, .	0.9	1
1713	Fully consistent density functional theory determination of the insulator-metal transition boundary in warm dense hydrogen. Physical Review Research, 2020, 2, .	1.3	15
1714	Accurate ab initio Description of Adsorption on Coordinatively Unsaturated Sites in Metalâ€“Organic Frameworks. , 2015, , 175-206.		3
1715	Van Der Waals Density Functionals for Graphene Layers and Graphite. Acta Physica Polonica A, 2011, 120, 845-848.	0.2	77
1716	STRUCTURAL, BONDING AND ELECTRONIC PROPERTIES OF BULK AND MONOLAYER INDIUM SELENIDE. Science Evolution, 2017, , 11-18.	0.1	2
1717	Reaction Mechanism for Methane-to-Methanol in Cu-SSZ-13: First-Principles Study of the Z2[Cu2O] and Z2[Cu2OH] Motifs. Catalysts, 2021, 11, 17.	1.6	2
1718	First Principles DFT Study of Hydrogen Storage on Graphene with La Decoration. Journal of Materials Science and Chemical Engineering, 2015, 03, 87-94.	0.2	3
1720	In-plane graphene/h-BN/graphene heterostructures with nanopores for electrical detection of DNA nucleotides. Physical Chemistry Chemical Physics, 2021, 23, 25126-25135.	1.3	5
1721	Application of Computational Chemistry for Contaminant Adsorption on the Components of Soil Surfaces. , 2022, , 171-213.		2
1722	Three-dimensional charge density wave observed by angle-resolved photoemission spectroscopy in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mo>Â</mml:mo> Physical Review B, 2021, 104, .	1.1	6
1723	Visualizing Spatial Evolution of Electron-Correlated Interface in Two-Dimensional Heterostructures. ACS Nano, 2021, 15, 16589-16596.	7.3	15

#	Article	IF	Citations
1724	A First-Principles Study of the Soft-Landing of $$mathrm{{Au}}_{16}$$ Au 16 on Graphite. Springer Theses, 2013, , 81-110.	0.0	0
1725	Application of (Kohnâ€“Sham) Density-Functional Theory to Real Materials. Letters in Mathematical Physics, 2014, , 191-206.	0.4	0
1726	10.3 Introduction to surface phonons. , 2015, , 586-615.		0
1727	Magnetic Properties of Ni/BN/Co Trilayer Structure: A First Principles Study. Journal of Magnetics, 2015, 20, 201-206.	0.2	0
1728	First-principles study of the phonon spectrum and heat capacity of TATB crystal. Wuli Xuebao/Acta Physica Sinica, 2016, 65, 126301.	0.2	5
1729	Determination of the total energy of a many-particle system. , 2018, , 28-37.		0
1730	Theoretical Methods of Surface Dynamics. Springer Series in Surface Sciences, 2018, , 117-142.	0.3	0
1732	First Principles Study of the Electronic Structure and Optical Properties of Pentacene under Pressure. Russian Journal of Physical Chemistry A, 2020, 94, 1040-1046.	0.1	0
1733	Uncertainty quantification in first-principles predictions of phonon properties and lattice thermal conductivity. Physical Review Materials, 2020, 4, .	0.9	2
1734	Tunable vertical ferroelectricity and domain walls by interlayer sliding in Î²-ZrI2. Npj Computational Materials, 2021, 7, .	3.5	14
1735	Designing xenes with two-dimensional triangular lattice. Physical Review Materials, 2020, 4, .	0.9	2
1736	Energetic Ground State Calculations, Electronic Band Structure at Surfaces. Springer Handbooks, 2020, , 471-498.	0.3	0
1737	Corrugated graphene exposes the limits of a widely used ab initio van der Waals DFT functional. Physical Review Materials, 2019, 3, .	0.9	2
1738	Ferroelectric critical size of SnTe nanoribbon and its mechanical strain engineering. Transactions of the JSME (in Japanese), 2020, 86, 19-00430-19-00430.	0.1	0
1739	Surface Phonons: Theoretical Methods and Results. Springer Handbooks, 2020, , 737-782.	0.3	2
1740	Energy Trends in Adsorption at Surfaces. , 2020, , 1321-1341.		1
1741	Establishing the accuracy of density functional approaches for the description of noncovalent interactions in ionic liquids. Physical Chemistry Chemical Physics, 2021, 23, 25558-25564.	1.3	5
1742	Adsorption of 2-Butanone on Pristine Graphene: A First-principles Study. VNU Journal of Science Mathematics - Physics, 2020, 36, .	0.0	4

#	Article	IF	Citations
1743	Applications of Current Density Functional Theory (DFT) Methods in Polymer Solar Cells. , 0, , .		0
1744	Theoretical Study of Weakly Bound Adsorbates on Au(111): Tests on van der Waals Density Functionals. Journal of Physical Chemistry C, 2021, 125, 24958-24966.	1.5	2
1745	Molecular Bond Engineering and Feature Learning for the Design of Hybrid Organicâ€“Inorganic Perovskite Solar Cells with Strong Noncovalent Halogenâ€“Cation Interactions. Journal of Physical Chemistry C, 2021, 125, 25316-25326.	1.5	6
1746	Stability threshold of formamidinium lead iodide determined by strain amplitudes. Journal Physics D: Applied Physics, 2020, 53, 504003.	1.3	1
1747	In pursuit of accurate interlayer potentials for twisted bilayer graphynes. Physical Chemistry Chemical Physics, 2021, 23, 27031-27041.	1.3	2
1748	Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory-Based Ab Initio Molecular Dynamics II: Extensions to the Isobaricâ€“Isoenthalpic and Isobaricâ€“Isothermal Ensembles. Journal of Chemical Theory and Computation, 2021, 17, 7789-7813.	2.3	7
1749	Density functional theory study of adsorption and diffusion of potassium atoms on zigzag graphene nanoribbons with different terminal groups. International Journal of Modern Physics B, 2021, 35, .	1.0	0
1750	Combining pressure and electrochemistry to synthesize superhydrides. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	11
1751	Structures and electronic properties of functional molecules on metal substrates: From single molecule to selfâ€assemblies. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1591.	6.2	3
1752	Evaluation of thermophysical properties of the LiCl-KCl system via ab initio and experimental methods. Journal of Nuclear Materials, 2022, 559, 153414.	1.3	13
1753	Phase Diagrams and Spectral Characteristics of Hydrofluorocarbon Hydrates: Insights from First-Principles Thermodynamics. ACS Sustainable Chemistry and Engineering, 2021, 9, 16347-16355.	3.2	3
1754	Recruiting Perovskites to Degrade Toxic Trinitrotoluene. Materials, 2021, 14, 7387.	1.3	5
1755	Exfoliating silica bilayers via intercalation at the silica/transition metal interface. Nanotechnology, 2022, 33, 135702.	1.3	0
1756	Spatial variation of geometry, binding, and electronic properties in the moirÃ© superstructure of MoS₂ on Au(111). 2D Materials, 2022, 9, 025003.	2.0	15
1757	Water Formation Reaction under Interfacial Confinement: Al0.25Si0.75O2 on O-Ru(0001). Nanomaterials, 2022, 12, 183.	1.9	2
1758	First-principles calculations of molecular adsorption on the surface of two-dimensional BCOH. Chemical Physics, 2022, 555, 111442.	0.9	1
1759	A DFT+U study on the adsorption of CO, H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>S, PH<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.svg"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>, CO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:msub><mml:mrow /><mml:	0.8	5
1762	The Electronic and Optical Properties of Vertically Stacked GaN-WS2 Heterostructure. Journal Wuhan University of Technology, Materials Science Edition, 2022, 37, 28-31.	0.4	1

#	Article	IF	Citations
1763	Dispersion interactions in proposed covalent superhydride superconductors. Physical Review B, 2022, 105, .	1.1	2
1764	Ab initio mechanistic insights into the stability, diffusion and storage capacity of sI clathrate hydrate containing hydrogen. International Journal of Hydrogen Energy, 2022, 47, 8419-8433.	3.8	10
1765	Study elastic properties of the leucine and isoleuicine from first principles calculations. Journal of Physics Condensed Matter, 2022, 34, 145702.	0.7	3
1766	Unraveling Heat Transport and Dissipation in Suspended MoSe₂ from Bulk to Monolayer. Advanced Materials, 2022, 34, e2108352.	11.1	12
1767	Stacking order and Coulomb correlation effect in the layered charge density wave phase of 1Tâ˜NbS2. Physical Review B, 2022, 105, .	1.1	13
1768	Engineering of the Topological Surface States and Topological Dangling Bond States in the (0001) Surface of Bi2Se3 via Structural Distortion. Physica Status Solidi (B): Basic Research, 2022, 259, .	0.7	1
1769	Linear response calculation with nonlocal van der Waals density functionals. Physical Review B, 2022, 105, .	1.1	3
1770	A new porphyrinic vanadium-based MOF constructed from infinite V(OH)O₄ chains: syntheses, characterization and photoabsorption properties. New Journal of Chemistry, 2022, 46, 632-641.	1.4	12
1771	Hard and soft materials: putting consistent van der Waals density functionals to work. Electronic Structure, 2022, 4, 014001.	1.0	4
1772	Copper-phthalocyanine (CuPc) and O, Li and Mn adatoms on graphene substrate: First-principles study of stability, magnetism and electronic properties. Surface Science, 2022, 719, 122023.	0.8	3
1773	First principle calculations including ab initio molecular dynamics studies for the activation of hydrogen fluoride on Ni(111). Chemical Physics, 2022, 557, 111469.	0.9	1
1774	Real-space detection and manipulation of two-dimensional quantum well states in few-layer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review B, 2022, 105, .	1.1	4
1775	Synergistic Mechanism of Combined Inhibitors on the Selective Flotation of Arsenopyrite and Pyrite. ACS Omega, 2022, 7, 6302-6312.	1.6	4
1776	Uniaxially Aligned 1D Sandwich-Molecular Wires: Electronic Structure and Magnetism. Journal of Physical Chemistry C, 2022, 126, 3140-3150.	1.5	4
1777	Capturing Individual Hydrogen Bond Strengths in Ices via Periodic Local Vibrational Mode Theory: Beyond the Lattice Energy Picture. Journal of Chemical Theory and Computation, 2022, 18, 562-579.	2.3	17
1778	Assessing density functionals for describing methane dissociative chemisorption on Pt(110)-(2Ã—1) surface. Chinese Journal of Chemical Physics, 2021, 34, 883-895.	0.6	2
1779	Binder-free S@Ti3C2Tx sandwich structure film as a high-capacity cathode for a stable aluminum-sulfur battery. Science China Materials, 2022, 65, 1463-1475.	3.5	20
1780	Predicting Biomolecule Adsorption on MoS₂ Nanosheets with High Structural Fidelity. Chemical Science, 0, , .	3.7	4

#	Article	IF	Citations
1781	Semi-empirical and linear-scaling DFT methods to characterize duplex DNA and G-quadruplexes in the presence of interacting small molecules. Physical Chemistry Chemical Physics, 2022, 24, 11510-11519.	1.3	5
1782	Untapped potential of 2D charge density wave chalcogenides as negative supercapacitor electrode materials. RSC Advances, 2022, 12, 6433-6439.	1.7	4
1783	Understanding the interactions between lithium polysulfides and anchoring materials in advanced lithiumâ€“sulfur batteries using density functional theory. Physical Chemistry Chemical Physics, 2022, 24, 8604-8623.	1.3	10
1784	Ground-state properties of the narrowest zigzag graphene nanoribbon from quantum Monte Carlo and comparison with density functional theory. Journal of Chemical Physics, 2022, 156, 084112.	1.2	4
1785	Partitioning of Atmospheric O₂ into High-pressure Ice in Ocean Worlds. Astrophysical Journal, 2022, 926, 72.	1.6	0
1786	Curly-Packed Structure Polymers for High-Temperature Capacitive Energy Storage. Chemistry of Materials, 2022, 34, 2333-2341.	3.2	25
1787	Hirshfeld atom refinement based on projector augmented wave densities with periodic boundary conditions. IUCrJ, 2022, 9, 286-297.	1.0	9
1788	Structure Evolution of Graphitic Surface upon Oxidation: Insights by Scanning Tunneling Microscopy. Jacs Au, 2022, 2, 723-730.	3.6	14
1789	Wide-Bandgap Perovskite Quantum Dots in Perovskite Matrix for Sky-Blue Light-Emitting Diodes. Journal of the American Chemical Society, 2022, 144, 4009-4016.	6.6	92
1790	High-Throughput Calculation of Interlayer van der Waals Forces Validated with Experimental Measurements. Research, 2022, 2022, 9765121.	2.8	10
1791	Neutron irradiation induced magnetization and persistent defects at high temperatures in graphite. Physical Review B, 2022, 105, .	1.1	1
1792	Towards Predicting the Sequential Appearance of Zeolitic Imidazolate Frameworks Synthesized by Mechanochemistry. Molecules, 2022, 27, 1946.	1.7	0
1793	Diffusion Monte Carlo Study on Relative Stabilities of Boron Nitride Polymorphs. Journal of Physical Chemistry C, 2022, 126, 6000-6007.	1.5	6
1794	Tunable band gap in twisted bilayer graphene. Physical Review B, 2022, 105, .	1.1	4
1795	An assessment of density functionals for predicting CO2 adsorption in diamine-functionalized metalâ€“organic frameworks. Journal of Chemical Physics, 2022, 156, 154113.	1.2	7
1796	Hypervalency in amorphous chalcogenides. Nature Communications, 2022, 13, 1458.	5.8	19
1797	Low Thermal Conductivity of Carbon Dioxide at High Pressure: Implications for Icy Planetary Interiors. Journal of Geophysical Research E: Planets, 2022, 127, .	1.5	4
1798	Quasi-Freestanding Bilayer Borophene on Ag(111). Nano Letters, 2022, 22, 3488-3494.	4.5	31

#	Article	IF	Citations
1799	Band offset trends in IVâ€“VI layered semiconductor heterojunctions. Journal of Physics Condensed Matter, 2022, 34, 195003.	0.7	3
1800	Visible Light-Driven Highly Selective CO₂ Reduction to CH₄ Using Potassium-Doped g-C₃N₅. Langmuir, 2022, 38, 3139-3148.	1.6	28
1801	Accounting for Dispersion Effects in the DFT Framework of Electrocatalysis: A Hybrid Solvation Model-Based Case Study of the Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2022, 126, 6171-6188.	1.5	3
1802	Dimerization of dehydrogenated polycyclic aromatic hydrocarbons on graphene. Journal of Chemical Physics, 2022, 156, 134703.	1.2	3
1803	Atomistic Insight into the Hydration States of Layered Double Hydroxides. ACS Omega, 2022, 7, 12412-12423.	1.6	9
1804	All carbon p-n border in bilayer graphene by the molecular orientation of intercalated corannulene. Journal of Applied Physics, 2022, 131, .	1.1	2
1805	Single-crystal graphene on Ir(110). Physical Review B, 2022, 105, .	1.1	7
1806	High-temperature phonon-mediated superconductivity in monolayer Mg2B4C2. Npj Quantum Materials, 2022, 7, .	1.8	11
1807	Towards accurate ionic relaxation algorithms for two-dimensional chalcogenide van der Waals materials - A first-principles study. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 140, 115223.	1.3	0
1808	Probabilistic deep learning approach for targeted hybrid organic-inorganic perovskites. Physical Review Materials, 2021, 5, .	0.9	5
1809	Accurate Simulations of the Reaction of H₂on a Curved Pt Crystal through Machine Learning. Journal of Physical Chemistry Letters, 2021, 12, 12157-12164.	2.1	5
1810	Emergence and Tuning of Multiple Flat Bands in Twisted Bilayer Î³-Graphyne. Journal of Physical Chemistry Letters, 2021, 12, 12283-12291.	2.1	3
1811	Theoretical study of stability, epitaxial formation, and phase transformations of two-dimensional pnictogen allotropes. Physical Review B, 2021, 104, .	1.1	3
1812	Density functional theory study of graphene adhesion on WX₂ (Xâ€‰=â€‰S and Se) monolayer: Role of atom vacancy and atomic reorganization defects. International Journal of Quantum Chemistry, 2022, 122, .	1.0	6
1813	Solidâ€State NMRâ€Driven Crystal Structure Prediction of Molecular Crystals: The Case of Mebendazole. Chemistry - A European Journal, 2022, 28, e202103589.	1.7	11
1814	Flexoelectricity Driven Fano Resonance in Slotted Carbon Nanotubes for Decoupled Multifunctional Sensing. Research, 2021, 2021, 9821905.	2.8	2
1815	An Ensemble Learning Platform for the Large-Scale Exploration of New Double Perovskites. ACS Applied Materials & Interfaces, 2022, 14, 717-725.	4.0	16
1816	Open-Shell Variant of the London Dispersion-Corrected Hartreeâ€“Fock Method (HFLD) for the Quantification and Analysis of Noncovalent Interaction Energies. Journal of Chemical Theory and Computation, 2022, 18, 2292-2307.	2.3	7

#	Article	IF	Citations
1817	Friction Behavior and Structural Evolution of Hexagonal Boron Nitride: A Relation to Environmental Molecules Containing â”OH Functional Group. ACS Applied Materials & Interfaces, 2022, 14, 19043-19055.	4.0	4
1818	Kinetics and energeticsÂof metal halide perovskite conversion reactions at the nanoscale. Communications Materials, 2022, 3, .	2.9	12
1819	Desorption of physisorbed molecular oxygen from coronene films and graphite surfaces. Journal of Chemical Physics, 0, , .	1.2	1
1821	Out-of-plane dipole-modulated photogenerated carrier separation and recombination at Janus-MoSSe/MoS₂ van der Waals heterostructure interfaces: an ab initio time-domain study. Physical Chemistry Chemical Physics, 2022, 24, 11743-11757.	1.3	2
1822	Organic ferroelectric croconic acid: a concise survey from bulk single crystals to thin films. Journal of Materials Chemistry C, 2022, 10, 8142-8167.	2.7	4
1823	Towards the rational design of Pt-based alloy catalysts for the low-temperature water-gas shift reaction: from extended surfaces to single atom alloys. Chemical Science, 2022, 13, 6385-6396.	3.7	9
1824	Anisotropy of thermal transport in phosphorene: A comparative first-principles study using different exchange-correlation functional. Materials Advances, 0, , .	2.6	0
1825	Size-limited high-density nanopore formation in two-dimensional moirÃ© materials. Physical Review B, 2022, 105, .	1.1	0
1826	Electronic band structure and chemical bonding in trigonal Se and Te. AIP Advances, 2022, 12, .	0.6	2
1827	Delving into guest-free and He-filled sI and sII clathrate hydrates: a first-principles computational study. Physical Chemistry Chemical Physics, 2022, 24, 13119-13129.	1.3	4
1828	Gasâ€Phase Errors Affect DFTâ€Based Electrocatalysis Models of Oxygen Reduction to Hydrogen Peroxide. ChemElectroChem, 2022, 9, .	1.7	2
1829	Ambiguous structure determination from powder data: four different structural models of 4,11-difluoroquinacridone with similar X-ray powder patterns, fit to the PDF, SSNMR and DFT-D. IUCrJ, 2022, 9, 406-424.	1.0	8
1830	Electronic and vibrational properties of bulk <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Cr</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> from first-principles calculations. Physical Review B, 2022, 105, .	1.1	0
1831	Insights into the Adsorption, Alloy Formation, and Poisoning Effects of Hg on Monometallic and Bimetallic Adsorbents. Langmuir, 0, , .	1.6	2
1832	Tribology at the atomic scale with density functional theory. Electronic Structure, 2022, 4, 023002.	1.0	3
1833	Grazing incidence fast atom and molecule diffraction: theoretical challenges. Physical Chemistry Chemical Physics, 2022, 24, 15628-15656.	1.3	3
1834	Accelerated Mining of 2D Van der Waals Heterojunctions by Integrating Supervised and Unsupervised Learning. Chemistry of Materials, 2022, 34, 5571-5583.	3.2	7
1835	Selecting the Reaction Path in On-Surface Synthesis through the Electron Chemical Potential in Graphene. Journal of the American Chemical Society, 2022, 144, 11003-11009.	6.6	2

#	Article	IF	Citations
1836	Pushing Down the Limit of NH₃ Detection of Graphene-Based Chemiresistive Sensors through Functionalization by Thermally Activated Tetrazoles Dimerization. ACS Nano, 2022, 16, 10456-10469.	7.3	8
1837	Design Traits for Diblock Copolymer Coating Properties on NaGdF₄ Upconversion Nanoparticles. ACS Applied Polymer Materials, 2022, 4, 5224-5233.	2.0	1
1838	Functional group contributions for azo derivatives as anode materials for KIBs: A first-principles study. Materials Chemistry and Physics, 2022, 289, 126430.	2.0	1
1839	Improved proton-transfer barriers with van der Waals density functionals: Role of repulsive non-local correlation. Journal of Chemical Physics, 2022, 156, .	1.2	3
1840	Carbon content drives high temperature superconductivity in a carbonaceous sulfur hydride below 100 GPa. Chemical Communications, 2022, 58, 9064-9067.	2.2	7
1841	Electrostatic properties of two-dimensional C₆₀ polymer thin films under an external electric field. Japanese Journal of Applied Physics, 2022, 61, 075004.	0.8	0
1842	Unraveling the Anchoring Effect of MXene-Supported Single Atoms as Cathodes for Aluminumâ€“Sulfur Batteries. , 2022, 4, 1436-1445.		11
1843	Rational Design of Synergistic Structure Between Single-Atoms and Nanoparticles for CO2 Hydrogenation to Formate Under Ambient Conditions. Frontiers in Chemistry, 0, 10, .	1.8	3
1844	Delocalization error: The greatest outstanding challenge in densityâ€functional theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	43
1845	Photoprotection in metal halide perovskites by ionic defect formation. Joule, 2022, 6, 2152-2174.	11.7	16
1846	A Career in Catalysis: Jens Kehlet NÃ¸rskov. ACS Catalysis, 2022, 12, 9679-9689.	5.5	19
1847	<tt>DMC-ICE13</tt>: Ambient and high pressure polymorphs of ice from diffusion Monte Carlo and density functional theory. Journal of Chemical Physics, 2022, 157, .	1.2	7
1848	A litmus test for the balanced description of dispersion interactions and coordination chemistry of lanthanoids. Physical Chemistry Chemical Physics, 0, , .	1.3	1
1849	Ï€â€Extended Zigzagâ€Shaped Diphenanthreneâ€Based pâ€Type Semiconductors Exhibiting Small Effective Masses. Advanced Electronic Materials, 2022, 8, .	2.6	1
1850	Nanoscale MXene Interlayer and Substrate Adhesion for Lubrication: A Density Functional Theory Study. ACS Applied Nano Materials, 2022, 5, 10516-10527.	2.4	28
1851	Deep Quantum-Dot Arrays in MoirÃ© Superlattices of Non-van der Waals Materials. Journal of the American Chemical Society, 2022, 144, 14657-14667.	6.6	3
1852	Effects of thermal, elastic, and surface properties on the stability of SiC polytypes. Physical Review B, 2022, 106, .	1.1	6
1853	Two-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:msub><mml:mi>Te</mml:mi><mml:mi><mml:n van der Waals heterostructures for tunnel-FET applications. Physical Review Materials, 2022, 6, .	3.1	8

#	Article	IF	Citations
1854	Workhorse minimally empirical dispersion-corrected density functional with tests for weakly bound systems: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msup><mml:mrow><mml:mi mathvariant="normal">r</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msup><mml:mi>SCAN</mml:mi><mml:mo>+</mml:mo> Physical Review B, 2022, 106, .	1.1	18
1855	Monodispersed FeS₂ Electrocatalyst Anchored to Nitrogenâ€Doped Carbon Host for Lithiumâ€“Sulfur Batteries. Advanced Functional Materials, 2022, 32, .	7.8	56
1856	Enhanced shift current bulk photovoltaic effect in ferroelectric Rashba semiconductor Î±-GeTe: ab initio study from three- to two-dimensional van der Waals layered structures. Journal of Physics Condensed Matter, 2022, 34, 435404.	0.7	1
1857	First- and second-order magneto-optical effects and intrinsically anomalous transport in the two-dimensional van der Waals layered magnets <mml:math		

#	Article	IF	Citations
1872	Ï€-Orbital mediated charge transfer channels in a monolayer Grâ€“NiPc heterointerface unveiled by soft X-ray electron spectroscopies and DFT calculations. Nanoscale, 2022, 14, 13166-13177.	2.8	2
1873	Computational investigation of van der Waals corrections in the adsorption properties of molecules on the Cu(111) surface. Physical Chemistry Chemical Physics, 2022, 24, 20294-20302.	1.3	3
1874	Van der Waals imprinting of black-phosphorus-like binary alloyed monolayers with tunable band gaps and moirÃ© superstructures. Physical Review B, 2022, 106, .	1.1	3
1875	Ion Conductivity in a Magnesium Borohydride Ammonia Borane Solid-State Electrolyte. Journal of Physical Chemistry C, 2022, 126, 15118-15127.	1.5	6
1876	Accurately Determining the Phase Transition Temperature of CsPbI₃ via Random-Phase Approximation Calculations and Phase-Transferable Machine Learning Potentials. Chemistry of Materials, 2022, 34, 8561-8576.	3.2	8
1877	Engineering chiral topological superconductivity in twisted Ising superconductors. Physical Review B, 2022, 106, .	1.1	2
1878	Electronâ€Transport Layers Employing Strongly Bound Ligands Enhance Stability in Colloidal Quantum Dot Infrared Photodetectors. Advanced Materials, 2022, 34, .	11.1	16
1879	Single- and Multilayers of Alkali Metal Atoms inside Graphene/MoS₂ Heterostructures: A Systematic First-Principles Study. Journal of Physical Chemistry C, 2022, 126, 15558-15564.	1.5	4
1880	Structural and charge transfer properties of ion intercalated 2D and bulk ice. Journal of Chemical Physics, 0, , .	1.2	0
1881	Hierarchal Porous Graphene-Structured Electrocatalysts with Feâ€“N₅ Active Sites Modified with Fe Clusters for Enhanced Performance Toward Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2022, 14, 42038-42047.	4.0	8
1882	An optimized smearing scheming for first Brillouin zone sampling and its application on thermal conductivity prediction of graphite. Chinese Physics B, 0, , .	0.7	0
1883	2D Dumbbell Silicene as a High Storage Capacity and Fast Ion Diffusion Anode for Li-Ion Batteries. ACS Applied Materials & Interfaces, 2022, 14, 47262-47271.	4.0	23
1884	Chemical Bonding With Plane Waves. , 2022, , .		2
1885	DFT based microkinetic modeling of confinement driven [4 + 2] Dielsâ€“Alder reactions between ethene and isoprene in H-ZSM5. Catalysis Science and Technology, 2022, 12, 7389-7407.	2.1	1
1886	How are Hydroxyl Groups Localized on a Graphene Sheet?. ACS Omega, 2022, 7, 37221-37228.	1.6	3
1887	Systematic Evaluation of Counterpoise Correction in Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 6742-6756.	2.3	20
1888	Effect of temperature on CO oxidation over Pt(111) in two-dimensional confinement. Journal of Chemical Physics, 2022, 157, 144701.	1.2	1
1889	Machine-learning accelerated identification of exfoliable two-dimensional materials. Machine Learning: Science and Technology, 2022, 3, 045014.	2.4	6

#	Article	IF	Citations
1890	Accurate Nonempirical Range-Separated Hybrid van der Waals Density Functional for Complex Molecular Problems, Solids, and Surfaces. Physical Review X, 2022, 12, .	2.8	5
1891	Photocatalytic activity of MoS₂ with water monolayers: Global optimization. Journal of Chemical Physics, 0, , .	1.2	1
1892	Tuning electronic and optical properties of monolayer MoS₂ by transition metal and nitrogen co-doping. Physica Scripta, 2022, 97, 115815.	1.2	4
1893	Active and selective reverse water-gas shift reaction over Pt/Na-Zeolite catalysts. Journal of CO2 Utilization, 2022, 66, 102291.	3.3	3
1894	First-principles calculations on O-atom diffusion on fluorinated graphene. Wuli Xuebao/Acta Physica Sinica, 2023, .	0.2	0
1895	Perspectives on weak interactions in complex materials at different length scales. Physical Chemistry Chemical Physics, 2023, 25, 2671-2705.	1.3	10
1896	Phonon Thermal Transport in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mi>Bi</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>Te</mml:mi><mml:m from a Deep-Neural-Network Interatomic Potential. Physical Review Applied, 2022, 18, .	1.5	9
1897	Functionalized electrodes embedded in nanopores: readâ€out enhancement?. Chemistry - an Asian Journal, 0, , .	1.7	1
1898	Macro superlubricity of two-dimensional disulphide/amorphous carbon heterogeneous via tribochemistry. Materials Today Nano, 2023, 21, 100286.	2.3	7
1899	Electrochemical Reduction of Carbon Dioxide at TiO₂/Au Nanocomposites. ACS Applied Materials & Interfaces, 2022, 14, 51889-51899.	4.0	9
1900	Efficient Method for the Computation of Frozen-Core Nuclear Gradients within the Random Phase Approximation. Journal of Chemical Theory and Computation, 2022, 18, 7359-7372.	2.3	5
1901	Elastic properties of moirÃ© lattices in epitaxial two-dimensional materials. Physical Review B, 2022, 106, .	1.1	2
1902	Hydrogenation of CO₂ to Methane over a Ru/RuTiO₂ Surface: A DFT Investigation into the Significant Role of the RuO₂ Overlayer. ACS Catalysis, 2022, 12, 14654-14666.	5.5	3
1903	Strong CO₂ Chemisorption in a Metalâ€“Organic Framework with Proximate Znâ€“OH Groups. Inorganic Chemistry, 2022, 61, 18710-18718.	1.9	1
1904	Electronic and magnetic properties of stacked graphene quantum dots. Diamond and Related Materials, 2023, 131, 109550.	1.8	4
1905	Band valley modification under strain in monolayer WSe2. AIP Advances, 2022, 12, .	0.6	4
1906	DFT calculations in solution systems: solvation energy, dispersion energy and entropy. Physical Chemistry Chemical Physics, 2023, 25, 913-931.	1.3	14
1907	Adsorption of aromatic molecules on a black phosphorene surface: a first-principles study. New Journal of Chemistry, 2023, 47, 1842-1851.	1.4	1

#	Article	IF	Citations
1908	Ab initio methods for the computation of physical properties and performance parameters of electrochemical energy storage devices. Physical Chemistry Chemical Physics, 2023, 25, 1476-1503.	1.3	3
1909	Interlayer and Intralayer Excitons in AlN/WS2 Heterostructure. Materials, 2022, 15, 8318.	1.3	2
1910	Strong Structural and Electronic Coupling in Metavalent PbS MoirÃ© Superlattices. Journal of the American Chemical Society, 2022, 144, 23474-23482.	6.6	1
1911	SBH17: Benchmark Database of Barrier Heights for Dissociative Chemisorption on Transition Metal Surfaces. Journal of Chemical Theory and Computation, 2023, 19, 245-270.	2.3	8
1912	Band valley flattening and exciton appearance/disappearance under isotropic strain in monolayer WS2. European Physical Journal Plus, 2022, 137, .	1.2	0
1913	Inhibiting the Laydown of Polymeric Carbon and Simultaneously Promoting Its Facile Burn-Off during the Industrial-Scale Production of Hydrogen with Nickel-Based Catalysts: Insights from Ab Initio Calculations. Nanomaterials, 2023, 13, 40.	1.9	0
1914	Mechanistic Insights on the Low-Temperature Oxidation of CO Catalyzed by Isolated Co Ions in N-Doped Carbon. ACS Catalysis, 2022, 12, 15529-15540.	5.5	1
1915	Interweaving Polar Charge Orders in a Layered Metallic Superatomic Crystal. Physical Review X, 2022, 12, .	2.8	0
1916	A â€œClickâ€•Reaction to Engineer MoS₂ Field-Effect Transistors with Low Contact Resistance. ACS Nano, 2022, 16, 20647-20655.	7.3	4
1917	Synthesis-on-substrate of quantum dot solids. Nature, 2022, 612, 679-684.	13.7	167
1918	Piezoelectric Response of Plastic Ionic Molecular Crystals: Role of Molecular Rotation. Crystal Growth and Design, 2023, 23, 729-740.	1.4	6
1919	Improving the Catalytic Performance of the Hydrogen Evolution Reaction of Î±â€MoB₂ via Rational Doping by Transition Metal Elements. ChemPhysChem, 2023, 24, .	1.0	1
1920	Interaction of organic pollutants with TiO₂: a density functional theory study of carboxylic acids on the anatase (101) surface. Molecular Physics, 0, , .	0.8	0
1921	Interface, vacancy, and morphology engineering synergistically improve In₂S₃@Cu₂S electrocatalytic performance for pH-universal HER. Journal of Materials Chemistry A, 2023, 11, 2262-2272.	5.2	10
1922	Biaxial Hard Compression, Anisotropic Elastic Property, and Pressure-Induced Isosymmetric Phase Transition in Ammonium Bicarbonate. Journal of Physical Chemistry C, 2023, 127, 831-841.	1.5	1
1923	Effect of Nickel on the Hydroxide Ion Adsorption of Copper Sulfide: A viewpoint from a first-principle calculation. Journal of Physics: Conference Series, 2023, 2421, 012011.	0.3	0
1924	Accuracy of Intermolecular interaction Energies, Particularly Those of Hetero Atom Containing Molecules Obtained by van der Waals DFT Calculations. ChemistrySelect, 2023, 8, .	0.7	1
1925	Spectroscopic Studies of Crystalline Neon Film Grown on a Gold Surface. Physics of Atomic Nuclei, 2022, 85, 1988-1991.	0.1	1

#	Article	IF	Citations
1926	Inorganic wide-bandgap perovskite subcells with dipole bridge for all-perovskite tandems. Nature Energy, 2023, 8, 610-620.	19.8	63
1927	Arsenic-Involving Intermolecular Interactions in Crystal Structures: The Dualistic Behavior of As(III) as Electron-Pair Donor and Acceptor. Crystal Growth and Design, 2023, 23, 1033-1048.	1.4	0
1928	High Ampacity On-Chip Wires Implemented by Aligned Carbon Nanotube-Cu Composite. Materials, 2023, 16, 1131.	1.3	0
1929	Effects of dispersion corrections on the theoretical description of bulk metals. Physical Review B, 2023, 107, .	1.1	5
1930	First-principles study of thermoelectric performance of monolayer Ge₂<i>X</i>₄S₂ (<i>X </i>= P, As). Wuli Xuebao/Acta Physica Sinica, 2023, 72, 077201.	0.2	0
1931	Propane Dehydrogenation on Pt_xSn_y (x, y â‰ 4) Clusters on Al₂O₃(110). ACS Catalysis, 2023, 13, 2802-2812.	5.5	13
1932	Zwitterionic or Not? Fast and Reliable Structure Determination by Combining Crystal Structure Prediction and Solid-State NMR. Molecules, 2023, 28, 1876.	1.7	0
1933	Expanding the low-dimensional interface engineering toolbox for efficient perovskite solar cells. Nature Energy, 2023, 8, 284-293.	19.8	23
1934	Rationalizing Functionalized MXenes as Effective Anchor Materials for Lithiumâ€“Sulfur Batteries via First-Principles Calculations. Journal of Physical Chemistry Letters, 2023, 14, 2215-2221.	2.1	4
1936	Superconductivity in Te-Deficient ZrTe₂. Journal of Physical Chemistry C, 2023, 127, 5162-5168.	1.5	2
1937	Smoothing Energy Transfer Enabling Efficient Largeâ€Area Quasiâ€2D Perovskite Lightâ€Emitting Diodes. Laser and Photonics Reviews, 2023, 17, .	4.4	1
1938	Simulating Highly Activated Sticking of H₂ on Al(110): Quantum versus Quasi-Classical Dynamics. Journal of Physical Chemistry C, 2023, 127, 5395-5407.	1.5	1
1939	Density functional theory and experimental study of multi-step lithiation in SnS2 anode. Ionics, 2023, 29, 1751-1763.	1.2	1
1940	Activation, Transportation, and Reaction of Alkyl Radicals on a Si(111)-B Surface by a Scanning Tunneling Microscope Tip. Journal of Physical Chemistry C, 2023, 127, 6002-6009.	1.5	0
1941	Thermal transport across flat and curved goldâ€“water interfaces: Assessing the effects of the interfacial modeling parameters. Journal of Chemical Physics, 2023, 158, .	1.2	4
1942	Evidence of Formation of 1â€“10 nm Diameter Ice Nanotubes in Double-Walled Carbon Nanotube Capillaries. ACS Nano, 2023, 17, 6922-6931.	7.3	5
1943	Gate-Induced Trans-Dimensionality of Carrier Distribution in Bilayer Lateral Heterosheet of MoS₂ and WS₂ for Semiconductor Devices with Tunable Functionality. ACS Applied Nano Materials, 2023, 6, 5434-5439.	2.4	2
1944	First principle study on transition metal ammine borohydrides with amphoteric hydrogen for hydrogen storage applications. International Journal of Hydrogen Energy, 2023, , .	3.8	0

#	Article	IF	Citations
1945	Large piezoelectric response in a Jahn-Teller distorted molecular metal halide. Nature Communications, 2023, 14, .	5.8	11
1946	Theoretical Study on the Electronic Properties of Two-Dimensional Covalent Triazine Frameworks/As van der Waals Heterostructures. Advances in Condensed Matter Physics, 2023, 2023, 1-8.	0.4	0
1947	Emergent charge density wave featuring quasi-one-dimensional chains in Ta-intercalated bilayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>2</mml:mn><mml:mi>H</mml:mi></mml:mrow><mml:m mathvariant="normal">Ta</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> with coexisting <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>2</mml:mn><mml:mtext>H-</mml:mtext></mml:mrow> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mrow><mml:msup> mathvariant="normal">T</mml:mi></mml:mrow><mml:mo>â€²</mml:mo></mml:msup><mml:mtext>â”</mml:mtext></mml:mrow> mathvariant="normal">MoTe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>	11.1	2
1948	Hydrogen-bond-bridged intermediate for perovskite solar cells with enhanced efficiency and stability. Nature Photonics, 2023, 17, 478-484.	15.6	62
1949	Understanding the wetting of transition metal dichalcogenides from an ab initio perspective. Physical Review Research, 2023, 5, .	1.3	0
1950	Theoretical Study on Origin of CVD Growth Direction Difference in Graphene/hBN Heterostructures. E-Journal of Surface Science and Nanotechnology, 2023, , .	0.1	0
1951	Elucidating the Effect of Ion Exchange Protocol on the Copper Exchange Efficacy, Copper Siting, and SCR activity in Cuâ€SSZâ€13. ChemPhysChem, 0, , .	1.0	0
1952	Contrasting electronic states of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>RuI</mml:mi><mml:mn>3</mml:mn></mml:msub></mml and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>RuCl</mml:mi><mml:mn>3</mml:mn></mml:msub></mml Physical Review B, 2023, 107, .	1.1	3
1953	Template-free scalable growth of vertically-aligned MoS₂ nanowire array meta-structural films towards robust superlubricity. Materials Horizons, 2023, 10, 4148-4162.	6.4	1
1968	Application of Molecular Simulation Methods in Treating Intrinsic Structures of Energetic Materials. , 2023, , 41-113.		1
1978	Review of Approximations for the Exchange-Correlation Energy in Density-Functional Theory. , 2023, , 1-90.		3
1984	Density Functional Theory Calculations for Materials with Complex Structures. The Materials Research Society Series, 2024, , 187-216.	0.2	0
2014			