Alexandre Tkatchenko

List of Publications by Year
in descending order

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205	29,789	8732 75	4750 169
papers	citations	h-index	g-index

214	214	214	20862
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Accurate Molecular Van Der Waals Interactions from Ground-State Electron Density and Free-Atom Reference Data. Physical Review Letters, 2009, 102, 073005.	2.9	4,824
2	Fast and Accurate Modeling of Molecular Atomization Energies with Machine Learning. Physical Review Letters, 2012, 108, 058301.	2.9	1,523
3	Accurate and Efficient Method for Many-Body van der Waals Interactions. Physical Review Letters, 2012, 108, 236402.	2.9	1,120
4	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
5	SchNet â€“ A deep learning architecture for molecules and materials. Journal of Chemical Physics, 2018, 148, 241722.	1.2	1,083
6	Quantum-chemical insights from deep tensor neural networks. Nature Communications, 2017, 8, 13890.	5.8	884
7	Machine learning of accurate energy-conserving molecular force fields. Science Advances, 2017, 3, e1603015.	4.7	695
8	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	1.2	589
9	Machine Learning Predictions of Molecular Properties: Accurate Many-Body Potentials and Nonlocality in Chemical Space. Journal of Physical Chemistry Letters, 2015, 6, 2326-2331.	2.1	575
10	Resolution-of-identity approach to Hartreeâ€“Fock, hybrid density functionals, RPA, MP2 andGWwith numeric atom-centered orbital basis functions. New Journal of Physics, 2012, 14, 053020.	1.2	549
11	Machine Learning Force Fields. Chemical Reviews, 2021, 121, 10142-10186.	23.0	528
12	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
13	Density-Functional Theory with Screened vanÂderÂWaals Interactions for the Modeling of Hybrid Inorganic-Organic Systems. Physical Review Letters, 2012, 108, 146103.	2.9	503
14	Assessment and Validation of Machine Learning Methods for Predicting Molecular Atomization Energies. Journal of Chemical Theory and Computation, 2013, 9, 3404-3419.	2.3	499
15	Machine learning of molecular electronic properties in chemical compound space. New Journal of Physics, 2013, 15, 095003.	1.2	482
16	Long-range correlation energy calculated from coupled atomic response functions. Journal of Chemical Physics, 2014, 140, 18A508.	1.2	480
17	Machine Learning for Molecular Simulation. Annual Review of Physical Chemistry, 2020, 71, 361-390.	4.8	456
18	Towards exact molecular dynamics simulations with machine-learned force fields. Nature Communications, 2018, 9, 3887.	5.8	452

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19	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	0.5	445
20	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
21	Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems. Chemical Reviews, 2021, 121, 9816-9872.	23.0	287
22	Stacking and Registry Effects in Layered Materials: The Case of Hexagonal Boron Nitride. Physical Review Letters, 2010, 105, 046801.	2.9	283
23	Unifying machine learning and quantum chemistry with a deep neural network for molecular wavefunctions. Nature Communications, 2019, 10, 5024.	5.8	282
24	Materials perspective on Casimir and van der Waals interactions. Reviews of Modern Physics, 2016, 88, .	16.4	276
25	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
26	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
27	Van der Waals Interactions Between Organic Adsorbates and at Organic/Inorganic Interfaces. MRS Bulletin, 2010, 35, 435-442.	1.7	257
28	Benzene adsorbed on metals: Concerted effect of covalency and van der Waals bonding. Physical Review B, 2012, 86, .	1.1	243
29	Scaling laws for van der Waals interactions in nanostructured materials. Nature Communications, 2013, 4, 2341.	5.8	243
30	SchNetPack: A Deep Learning Toolbox For Atomistic Systems. Journal of Chemical Theory and Computation, 2019, 15, 448-455.	2.3	240
31	Dispersion-corrected MÃ¸llerâ€“Plesset second-order perturbation theory. Journal of Chemical Physics, 2009, 131, 094106.	1.2	223
32	i-PI 2.0: A universal force engine for advanced molecular simulations. Computer Physics Communications, 2019, 236, 214-223.	3.0	220
33	Modeling Adsorption and Reactions of Organic Molecules at Metal Surfaces. Accounts of Chemical Research, 2014, 47, 3369-3377.	7.6	218
34	Wavelike charge density fluctuations and van der Waals interactions at the nanoscale. Science, 2016, 351, 1171-1176.	6.0	217
35	On the accuracy of density-functional theory exchange-correlation functionals for H bonds in small water clusters. II. The water hexamer and van der Waals interactions. Journal of Chemical Physics, 2008, 129, 194111.	1.2	211
36	Two- and three-body interatomic dispersion energy contributions to binding in molecules and solids. Journal of Chemical Physics, 2010, 132, 234109.	1.2	194

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37	Hydrogen Bonds and van der Waals Forces in Ice at Ambient and High Pressures. Physical Review Letters, 2011, 107, 185701.	2.9	193
38	Beyond the Random-Phase Approximation for the Electron Correlation Energy: The Importance of Single Excitations. Physical Review Letters, 2011, 106, 153003.	2.9	193
39	Many-body van der Waals interactions in molecules and condensed matter. Journal of Physics Condensed Matter, 2014, 26, 213202.	0.7	190
40	Performance of various density-functional approximations for cohesive properties of 64 bulk solids. New Journal of Physics, 2018, 20, 063020.	1.2	185
41	Exploring chemical compound space with quantum-based machine learning. Nature Reviews Chemistry, 2020, 4, 347-358.	13.8	184
42	Collective many-body van der Waals interactions in molecular systems. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 14791-14795.	3.3	178
43	van der Waals dispersion interactions in molecular materials: beyond pairwise additivity. Chemical Science, 2015, 6, 3289-3301.	3.7	172
44	Adsorption Geometry Determination of Single Molecules by Atomic Force Microscopy. Physical Review Letters, 2013, 111, 106103.	2.9	162
45	Hard Numbers for Large Molecules: Toward Exact Energetics for Supramolecular Systems. Journal of Physical Chemistry Letters, 2014, 5, 849-855.	2.1	159
46	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
47	Role of Dispersion Interactions in the Polymorphism and Entropic Stabilization of the Aspirin Crystal. Physical Review Letters, 2014, 113, 055701.	2.9	156
48	Manyâ€Body Dispersion Interactions in Molecular Crystal Polymorphism. Angewandte Chemie - International Edition, 2013, 52, 6629-6632.	7.2	149
49	Understanding Molecular Crystals with Dispersion-Inclusive Density Functional Theory: Pairwise Corrections and Beyond. Accounts of Chemical Research, 2014, 47, 3208-3216.	7.6	146
50	van der Waals Interactions in Ionic and Semiconductor Solids. Physical Review Letters, 2011, 107, 245501.	2.9	143
51	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
52	Firstâ€principles modeling of molecular crystals: structures and stabilities, temperature and pressure. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1294.	6.2	141
53	sGDML: Constructing accurate and data efficient molecular force fields using machine learning. Computer Physics Communications, 2019, 240, 38-45.	3.0	137
54	Non-covalent interactions across organic and biological subsets of chemical space: Physics-based potentials parametrized from machine learning. Journal of Chemical Physics, 2018, 148, 241706.	1.2	136

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55	Interatomic methods for the dispersion energy derived from the adiabatic connection fluctuation-dissipation theorem. Journal of Chemical Physics, 2013, 138, 074106.	1.2	129
56	Reliable and practical computational description of molecular crystal polymorphs. Science Advances, 2019, 5, eaau3338.	4.7	127
57	Sliding Mechanisms in Multilayered Hexagonal Boron Nitride and Graphene: The Effects of Directionality, Thickness, and Sliding Constraints. Physical Review Letters, 2015, 114, 096101.	2.9	121
58	Adsorption structures and energetics of molecules on metal surfaces: Bridging experiment and theory. Progress in Surface Science, 2016, 91, 72-100.	3.8	121
59	Machine Learning Force Fields and Coarse-Grained Variables in Molecular Dynamics: Application to Materials and Biological Systems. Journal of Chemical Theory and Computation, 2020, 16, 4757-4775.	2.3	120
60	Seamless and Accurate Modeling of Organic Molecular Materials. Journal of Physical Chemistry Letters, 2013, 4, 1028-1033.	2.1	119
61	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
62	Machine learning for chemical discovery. Nature Communications, 2020, 11, 4125.	5.8	117
63	Theory and practice of modeling van der Waals interactions in electronic-structure calculations. Chemical Society Reviews, 2019, 48, 4118-4154.	18.7	114
64	Describing Both Dispersion Interactions and Electronic Structure Using Density Functional Theory: The Case of Metalâ^'Phthalocyanine Dimers. Journal of Chemical Theory and Computation, 2010, 6, 81-90.	2.3	109
65	First-Principles Modeling of Non-Covalent Interactions in Supramolecular Systems: The Role of Many-Body Effects. Journal of Chemical Theory and Computation, 2012, 8, 4317-4322.	2.3	104
66	Current Understanding of Van der Waals Effects in Realistic Materials. Advanced Functional Materials, 2015, 25, 2054-2061.	7.8	101
67	Unraveling the Stability of Polypeptide Helices: Critical Role of van der Waals Interactions. Physical Review Letters, 2011, 106, 118102.	2.9	97
68	Powder diffraction and crystal structure prediction identify four new coumarin polymorphs. Chemical Science, 2017, 8, 4926-4940.	3.7	97
69	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
70	Quantitative Prediction of Molecular Adsorption: Structure and Binding of Benzene on Coinage Metals. Physical Review Letters, 2015, 115, 036104.	2.9	89
71	Advances in Density-Functional Calculations for Materials Modeling. Annual Review of Materials Research, 2019, 49, 1-30.	4.3	87
72	Molecular switches from benzene derivatives adsorbed on metal surfaces. Nature Communications, 2013, 4, 2569.	5.8	82

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73	Molecular force fields with gradient-domain machine learning: Construction and application to dynamics of small molecules with coupled cluster forces. Journal of Chemical Physics, 2019, 150, 114102.	1.2	81
74	Electronic Properties of Molecules and Surfaces with a Self-Consistent Interatomic van der Waals Density Functional. Physical Review Letters, 2015, 114, 176802.	2.9	79
75	Popular Kohn-Sham density functionals strongly overestimate many-body interactions in van der Waals systems. Physical Review B, 2008, 78, .	1.1	75
76	Noncovalent Interactions of DNA Bases with Naphthalene and Graphene. Journal of Chemical Theory and Computation, 2013, 9, 2090-2096.	2.3	73
77	Many-body dispersion effects in the binding of adsorbates on metal surfaces. Journal of Chemical Physics, 2015, 143, 102808.	1.2	69
78	Nanoscale Ï€â€“Ï€ stacked molecules are bound by collective charge fluctuations. Nature Communications, 2017, 8, 14052.	5.8	69
79	Fast and accurate quantum Monte Carlo for molecular crystals. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 1724-1729.	3.3	69
80	Non-additivity of molecule-surface van der Waals potentials from force measurements. Nature Communications, 2014, 5, 5568.	5.8	65
81	van der Waals Interactions Determine Selectivity in Catalysis by Metallic Gold. Journal of the American Chemical Society, 2014, 136, 13333-13340.	6.6	63
82	Understanding the Structure and Electronic Properties of Molecular Crystals Under Pressure: Application of Dispersion Corrected DFT to Oligoacenes. Journal of Physical Chemistry A, 2013, 117, 8323-8331.	1.1	61
83	Many-Body Descriptors for Predicting Molecular Properties with Machine Learning: Analysis of Pairwise and Three-Body Interactions in Molecules. Journal of Chemical Theory and Computation, 2018, 14, 2991-3003.	2.3	59
84	Machine Learning Force Fields: Recent Advances and Remaining Challenges. Journal of Physical Chemistry Letters, 2021, 12, 6551-6564.	2.1	58
85	Interactions between large molecules pose a puzzle for reference quantum mechanical methods. Nature Communications, 2021, 12, 3927.	5.8	57
86	Understanding non-covalent interactions in larger molecular complexes from first principles. Journal of Chemical Physics, 2019, 150, 010901.	1.2	56
87	Accurate Many-Body Repulsive Potentials for Density-Functional Tight Binding from Deep Tensor Neural Networks. Journal of Physical Chemistry Letters, 2020, 11, 6835-6843.	2.1	55
88	Density Functional Model for van der Waals Interactions: Unifying Many-Body Atomic Approaches with Nonlocal Functionals. Physical Review Letters, 2020, 124, 146401.	2.9	53
89	Quantitative Prediction of Optical Absorption in Molecular Solids from an Optimally Tuned Screened Range-Separated Hybrid Functional. Journal of Chemical Theory and Computation, 2018, 14, 2919-2929.	2.3	51
90	Exploring the bonding of large hydrocarbons on noble metals: Diindoperylene on Cu(111), Ag(111), and Au(111). Physical Review B, 2013, 87, .	1.1	49

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91	Capturing intensive and extensive DFT/TDDFT molecular properties with machine learning. European Physical Journal B, 2018, 91, 1.	0.6	48
92	QM7-X, a comprehensive dataset of quantum-mechanical properties spanning the chemical space of small organic molecules. Scientific Data, 2021, 8, 43.	2.4	46
93	Adsorption of Ar on graphite using London dispersion forces corrected Kohn-Sham density functional theory. Physical Review B, 2006, 73, .	1.1	43
94	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
95	Noncovalent Bonding Controls Selectivity in Heterogeneous Catalysis: Coupling Reactions on Gold. Journal of the American Chemical Society, 2016, 138, 15243-15250.	6.6	43
96	Properties of the water to boron nitride interaction: From zero to two dimensions with benchmark accuracy. Journal of Chemical Physics, 2017, 147, 044710.	1.2	43
97	Role of methyl-induced polarization in ion binding. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 12978-12983.	3.3	42
98	Quantum tunneling of thermal protons through pristine graphene. Journal of Chemical Physics, 2018, 148, 204707.	1.2	42
99	Electronic structure of dye-sensitized TiO<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>clusters from many-body perturbation theory. Physical Review B, 2011, 84, .	1.1	41
100	Catalysis beyond frontier molecular orbitals: Selectivity in partial hydrogenation of multi-unsaturated hydrocarbons on metal catalysts. Science Advances, 2017, 3, e1700939.	4.7	41
101	Electrodynamic response and stability of molecular crystals. Physical Review B, 2013, 87, .	1.1	40
102	Quantum-Mechanical Relation between Atomic Dipole Polarizability and the van der Waals Radius. Physical Review Letters, 2018, 121, 183401.	2.9	40
103	First-principles stability ranking of molecular crystal polymorphs with the DFT+MBD approach. Faraday Discussions, 2018, 211, 253-274.	1.6	39
104	Computational polymorph screening reveals late-appearing and poorly-soluble form of rotigotine. Communications Chemistry, 2019, 2, .	2.0	39
105	Quantum mechanics of proteins in explicit water: The role of plasmon-like solute-solvent interactions. Science Advances, 2019, 5, eaax0024.	4.7	39
106	Mechanical and Tribological Properties of Layered Materials under High Pressure: Assessing the Importance of Many-Body Dispersion Effects. Journal of Chemical Theory and Computation, 2020, 16, 666-676.	2.3	39
107	Electronic Structure and van der Waals Interactions in the Stability and Mobility of Point Defects in Semiconductors. Physical Review Letters, 2013, 111, 045501.	2.9	37
108	Structure and Stability of Molecular Crystals with Many-Body Dispersion-Inclusive Density Functional Tight Binding. Journal of Physical Chemistry Letters, 2018, 9, 399-405.	2.1	37

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109	Understanding Structure and Bonding of Multilayered Metalâ€“Organic Nanostructures. Journal of Physical Chemistry C, 2013, 117, 3055-3061.	1.5	36
110	Physical adsorption at the nanoscale: Towards controllable scaling of the substrate-adsorbate van der Waals interaction. Physical Review B, 2017, 95, .	1.1	36
111	Structure and Formation of Synthetic Hemozoin: Insights From First-Principles Calculations. Crystal Growth and Design, 2011, 11, 3332-3341.	1.4	34
112	Toward Low-Temperature Dehydrogenation Catalysis: Isophorone Adsorbed on Pd(111). Journal of Physical Chemistry Letters, 2012, 3, 582-586.	2.1	33
113	Modeling quantum nuclei with perturbed path integral molecular dynamics. Chemical Science, 2016, 7, 1368-1372.	3.7	31
114	Long-Range Repulsion Between Spatially Confined van der Waals Dimers. Physical Review Letters, 2017, 118, 210402.	2.9	31
115	Quantitative imaging of electric surface potentials with single-atom sensitivity. Nature Materials, 2019, 18, 853-859.	13.3	31
116	Molecular basis for higher affinity of <scp>SARSâ€CoV</scp>â€2 spike <scp>RBD</scp> for human <scp>ACE2</scp> receptor. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1134-1144.	1.5	31
117	Interpolating Nonadiabatic Molecular Dynamics Hamiltonian with Artificial Neural Networks. Journal of Physical Chemistry Letters, 2021, 12, 6070-6077.	2.1	29
118	BIGDMLâ€”Towards accurate quantum machine learning force fields for materials. Nature Communications, 2022, 13, .	5.8	29
119	Benzene adsorbed on Si(001): The role of electron correlation and finite temperature. Physical Review B, 2012, 85, .	1.1	28
120	Size Effects in the Interface Level Alignment of Dye-Sensitized TiO₂ Clusters. Journal of Physical Chemistry Letters, 2014, 5, 2395-2401.	2.1	28
121	Thermal and Electronic Fluctuations of Flexible Adsorbed Molecules: Azobenzene on Ag(111). Physical Review Letters, 2016, 116, 146101.	2.9	26
122	Unifying Microscopic and Continuum Treatments of van der Waals and Casimir Interactions. Physical Review Letters, 2017, 118, 266802.	2.9	25
123	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
124	Molecular force fields with gradient-domain machine learning (GDML): Comparison and synergies with classical force fields. Journal of Chemical Physics, 2020, 153, 124109.	1.2	25
125	Dynamical strengthening of covalent and non-covalent molecular interactions by nuclear quantum effects at finite temperature. Nature Communications, 2021, 12, 442.	5.8	25
126	Quantum-Chemical Insights from Interpretable Atomistic Neural Networks. Lecture Notes in Computer Science, 2019, , 311-330.	1.0	25

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127	Machine learning of material properties: Predictive and interpretable multilinear models. Science Advances, 2022, 8, eabm7185.	4.7	25
128	Challenges for machine learning force fields in reproducing potential energy surfaces of flexible molecules. Journal of Chemical Physics, 2021, 154, 094119.	1.2	24
129	Tailoring van der Waals dispersion interactions with external electric charges. Nature Communications, 2018, 9, 3017.	5.8	23
130	Pair-Wise and Many-Body Dispersive Interactions Coupled to an Optimally Tuned Range-Separated Hybrid Functional. Journal of Chemical Theory and Computation, 2013, 9, 3473-3478.	2.3	22
131	High-Throughput Investigation of the Geometry and Electronic Structures of Gas-Phase and Crystalline Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry C, 2014, 118, 19964-19974.	1.5	22
132	Identical Binding Energies and Work Functions for Distinct Adsorption Structures: Olympicenes on the Cu(111) Surface. Journal of Physical Chemistry Letters, 2016, 7, 1022-1027.	2.1	22
133	Phase transition between cubic and monoclinic polymorphs of the tetracyanoethylene crystal: the role of temperature and kinetics. CrystEngComm, 2012, 14, 4656.	1.3	21
134	From quantum to continuum mechanics in the delamination of atomically-thin layers from substrates. Nature Communications, 2020, 11, 1651.	5.8	21
135	Coulomb interactions between dipolar quantum fluctuations in van der Waals bound molecules and materials. Nature Communications, 2021, 12, 137.	5.8	21
136	Charge transfer and adsorption energies in the iodineâ€“Pt(111) interaction. Surface Science, 2005, 581, 58-65.	0.8	20
137	RuppetÂal.Reply:. Physical Review Letters, 2012, 109, .	2.9	20
138	Binding energies of benzene on coinage metal surfaces: Equal stability on different metals. Journal of Chemical Physics, 2018, 148, 214703.	1.2	20
139	Four-Dimensional Scaling of Dipole Polarizability in Quantum Systems. Physical Review Letters, 2022, 128, 070602.	2.9	20
140	Commensurate monolayers on surfaces: Geometry and ground states. Physical Review B, 2007, 75, .	1.1	19
141	Steps or Terraces? Dynamics of Aromatic Hydrocarbons Adsorbed at Vicinal Metal Surfaces. Physical Review Letters, 2015, 115, 086101.	2.9	19
142	Adsorption of isophorone and trimethyl-cyclohexanone on Pd(111): A combination of infrared reflection absorption spectroscopy and density functional theory studies. Surface Science, 2016, 650, 149-160.	0.8	19
143	Strong Local-Field Enhancement of the Nonlinear Soft-Mode Response in a Molecular Crystal. Physical Review Letters, 2017, 119, 097404.	2.9	19
144	Improving molecular force fields across configurational space by combining supervised and unsupervised machine learning. Journal of Chemical Physics, 2021, 154, 124102.	1.2	19

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145	Hidden Beneath the Surface: Origin of the Observed Enantioselective Adsorption on PdGa(111). Journal of the American Chemical Society, 2018, 140, 1401-1408.	6.6	16
146	Electronic charge rearrangement at metal/organic interfaces induced by weak van der Waals interactions. Physical Review Materials, 2017, 1, .	0.9	16
147	Fine-Structure Constant Connects Electronic Polarizability and Geometric van-der-Waals Radius of Atoms. Journal of Physical Chemistry Letters, 2021, 12, 9488-9492.	2.1	15
148	Interaction of Isophorone with Pd(111): A Combination of Infrared Reflectionâ€“Absorption Spectroscopy, Near-Edge X-ray Absorption Fine Structure, and Density Functional Theory Studies. Journal of Physical Chemistry C, 2014, 118, 27833-27842.	1.5	14
149	Tuning the work function of stepped metal surfaces by adsorption of organic molecules. Journal of Physics Condensed Matter, 2017, 29, 204001.	0.7	14
150	Stability of functionalized platform molecules on Au(111). Journal of Chemical Physics, 2018, 149, 244705.	1.2	14
151	Nonadditivity of the Adsorption Energies of Linear Acenes on Au(111): Molecular Anisotropy and Many-Body Effects. Journal of Physical Chemistry Letters, 2019, 10, 1000-1004.	2.1	14
152	Colossal Enhancement of Atomic Force Response in van der Waals Materials Arising from Many-Body Electronic Correlations. Physical Review Letters, 2022, 128, 106101.	2.9	14
153	Nature of Hydrogen Bonds and SÂ·Â·Â·S Interactions in the <scp>l</scp>-Cystine Crystal. Journal of Physical Chemistry A, 2016, 120, 4223-4230.	1.1	13
154	Phonon-Polariton Mediated Thermal Radiation and Heat Transfer among Molecules and Macroscopic Bodies: Nonlocal Electromagnetic Response at Mesoscopic Scales. Physical Review Letters, 2018, 121, 045901.	2.9	13
155	Ion-Hydroxyl Interactions: From High-Level Quantum Benchmarks to Transferable Polarizable Force Fields. Journal of Chemical Theory and Computation, 2019, 15, 2444-2453.	2.3	13
156	Optical van-der-Waals forces in molecules: from electronic Bethe-Salpeter calculations to the many-body dispersion model. Nature Communications, 2022, 13, 813.	5.8	13
157	Potential Energy Landscape of Monolayer-Surface Systems Governed by Repulsive Lateral Interactions: The Case of(3Ã—3)â^'Iâ^'Pt(111). Physical Review Letters, 2006, 97, 036102.	2.9	12
158	First-Principles Study of Alkoxides Adsorbed on Au(111) and Au(110) Surfaces: Assessing the Roles of Noncovalent Interactions and Molecular Structures in Catalysis. Journal of Physical Chemistry C, 2017, 121, 27905-27914.	1.5	12
159	Anisotropic Interlayer Force Field for Transition Metal Dichalcogenides: The Case of Molybdenum Disulfide. Journal of Chemical Theory and Computation, 2021, 17, 7237-7245.	2.3	12
160	Communication: Many-body stabilization of non-covalent interactions: Structure, stability, and mechanics of Ag3Co(CN)6 framework. Journal of Chemical Physics, 2016, 145, 241101.	1.2	11
161	Improved description of ligand polarization enhances transferability of ionâ€“ligand interactions. Journal of Chemical Physics, 2020, 153, 094115.	1.2	11
162	Quantum framework for describing retarded and nonretarded molecular interactions in external electric fields. Physical Review Research, 2022, 4, .	1.3	11

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163	Significance of the Chemical Environment of an Element in Nonadiabatic Molecular Dynamics: Feature Selection and Dimensionality Reduction with Machine Learning. Journal of Physical Chemistry Letters, 2021, 12, 12026-12032.	2.1	11
164	Analytic theory of hexagonal monolayer interacting with hexagonal substrate. Physical Review B, 2006, 74, .	1.1	10
165	Effective scheme to determine accurate defect formation energies and charge transition levels of point defects in semiconductors. Physical Review B, 2017, 96, .	1.1	10
166	Uniaxial negative thermal expansion and metallophilicity in Cu3[Co(CN)6]. Journal of Solid State Chemistry, 2018, 258, 298-306.	1.4	10
167	Perturbed path integrals in imaginary time: Efficiently modeling nuclear quantum effects in molecules and materials. Journal of Chemical Physics, 2018, 148, 102325.	1.2	10
168	Subtle Fluorination of Conjugated Molecules Enables Stable Nanoscale Assemblies on Metal Surfaces. Journal of Physical Chemistry C, 2018, 122, 18902-18911.	1.5	10
169	Terahertz spectroscopy of 2,4,6-trinitrotoluene molecular solids from first principles. Beilstein Journal of Organic Chemistry, 2018, 14, 381-388.	1.3	10
170	Construction of Machine Learned Force Fields with Quantum Chemical Accuracy: Applications and Chemical Insights. Lecture Notes in Physics, 2020, , 277-307.	0.3	10
171	Adsorption site, core level shifts and charge transfer on the Pd(111)â€“I(âˆš3Ã—âˆš3) surface. Surface Science, 2006, 600, 3093-3098.	0.8	9
172	Tuning Intermolecular Interactions with Nanostructured Environments. Chemistry of Materials, 2017, 29, 2452-2458.	3.2	9
173	Predictive QM/MM Modeling of Modulations in Proteinâ€“Protein Binding by Lysine Methylation. Journal of Molecular Biology, 2021, 433, 166745.	2.0	9
174	Quantum-mechanical force balance between multipolar dispersion and Pauli repulsion in atomic van der Waals dimers. Physical Review Research, 2021, 3, .	1.3	9
175	Detailed characterization of (3Ã—3) iodine adlayer on Pt(111) by unequal-sphere packing model. Journal of Chemical Physics, 2005, 122, 094705.	1.2	8
176	Unequal-sphere packing model for the structural arrangement of the well-ordered adsorbate-substrate system. Physical Review B, 2004, 70, .	1.1	7
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