Giulia Galli

List of Publications by Year
in descending order

178 papers	11,000 citations	25031 57 h-index	33889 99 g-index
182 all docs	182 docs citations	182 times ranked	12114 citing authors

#	Article	IF	Citations
1	Photoelectron spectra of water and simple aqueous solutions at extreme conditions. Faraday Discussions, 2022, , .	3.2	1
2	Five-second coherence of a single spin with single-shot readout in silicon carbide. Science Advances, 2022, 8, eabm5912.	10.3	57
3	Quantum simulations of thermally activated delayed fluorescence in an all-organic emitter. Physical Chemistry Chemical Physics, 2022, 24, 10101-10113.	2.8	6
4	Determining the Oxygen Stoichiometry of Cobaltite Thin Films. Chemistry of Materials, 2022, 34, 2076-2084.	6.7	2
5	Simulating the Electronic Structure of Spin Defects on Quantum Computers. PRX Quantum, 2022, 3, .	9.2	18
6	Generalized scaling of spin qubit coherence in over 12,000 host materials. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2121808119.	7.1	38
7	Understanding the Effect of Lead Iodide Excess on the Performance of Methylammonium Lead Iodide Perovskite Solar Cells. ACS Energy Letters, 2022, 7, 1912-1919.	17.4	14
8	Greenâ€™s Function Formulation of Quantum Defect Embedding Theory. Journal of Chemical Theory and Computation, 2022, 18, 3512-3522.	5.3	17
9	Influence of nuclear quantum effects on the electronic properties of amorphous carbon. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	7
10	Probing the Coherence of Solid-State Qubits at Avoided Crossings. PRX Quantum, 2021, 2, .	9.2	29
11	The impact of surface composition on the interfacial energetics and photoelectrochemical properties of BiVO4. Nature Energy, 2021, 6, 287-294.	39.5	108
12	Molecular Polarizabilities in Aqueous Systems from First-Principles. Journal of Physical Chemistry B, 2021, 125, 2183-2192.	2.6	4
13	Determining the Structureâ€“Property Relationships of Quasi-Two-Dimensional Semiconductor Nanoplatelets. Journal of Physical Chemistry C, 2021, 125, 4820-4827.	3.1	7
14	Code interoperability extends the scope of quantum simulations. Npj Computational Materials, 2021, 7, .	8.7	8
15	Quantum Embedding Theory for Strongly Correlated States in Materials. Journal of Chemical Theory and Computation, 2021, 17, 2116-2125.	5.3	45
16	Solvation of simple ions in water at extreme conditions. Journal of Chemical Physics, 2021, 154, 144501.	3.0	6
17	Predicting the Onset of Metalâ€“Insulator Transitions in Transition Metal Oxidesâ€”A First Step in Designing Neuromorphic Devices. Chemistry of Materials, 2021, 33, 3187-3195.	6.7	9
18	Quantum guidelines for solid-state spin defects. Nature Reviews Materials, 2021, 6, 906-925.	48.7	185

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19	Substrate-controlled dynamics of spin qubits in low dimensional van der Waals materials. Applied Physics Letters, 2021, 118, .	3.3	9
20	Lessons learned from first-principles calculations of transition metal oxides. Journal of Chemical Physics, 2021, 154, 174704.	3.0	5
21	Integration of theory and experiment in the modelling of heterogeneous electrocatalysis. Nature Energy, 2021, 6, 700-705.	39.5	42
22	Cation and anion topotactic transformations in cobaltite thin films leading to Ruddlesden-Popper phases. Physical Review Materials, 2021, 5, .	2.4	7
23	Advanced Materials for Energy-Water Systems: The Central Role of Water/Solid Interfaces in Adsorption, Reactivity, and Transport. Chemical Reviews, 2021, 121, 9450-9501.	47.7	43
24	Spinâ€“spin interactions in defects in solids from mixed all-electron and pseudopotential first-principles calculations. Npj Computational Materials, 2021, 7, .	8.7	12
25	Theoretical and experimental study of the nitrogen-vacancy center in 4H-SiC. Physical Review Materials, 2021, 5, .	2.4	6
26	Quantum vibronic effects on the electronic properties of solid and molecular carbon. Physical Review Materials, 2021, 5, .	2.4	12
27	Spatial Patterns of Light-Harvesting Antenna Complex Arrangements Tune the Transfer-to-Trap Efficiency of Excitons in Purple Bacteria. Journal of Physical Chemistry Letters, 2021, 12, 6967-6973.	4.6	2
28	Photoluminescence spectra of point defects in semiconductors: Validation of first-principles calculations. Physical Review Materials, 2021, 5, .	2.4	29
29	Observation of spatially resolved Rashba states on the surface of CH3NH3PbBr3 single crystals. Applied Physics Reviews, 2021, 8, .	11.3	12
30	First-Principles Predictions of Out-of-Plane Group IV and V Dimers as High-Symmetry, High-Spin Defects in Hexagonal Boron Nitride. ACS Applied Materials & Interfaces, 2021, 13, 45768-45777.	8.0	12
31	Machine learning dielectric screening for the simulation of excited state properties of molecules and materials. Chemical Science, 2021, 12, 4970-4980.	7.4	16
32	Integrating Computation and Experiment to Investigate Photoelectrodes for Solar Water Splitting at the Microscopic Scale. Accounts of Chemical Research, 2021, 54, 3863-3872.	15.6	7
33	PyCCE: A Python Package for Cluster Correlation Expansion Simulations of Spin Qubit Dynamics. Advanced Theory and Simulations, 2021, 4, 2100254.	2.8	14
34	Probing the electronic properties of the electrified silicon/water interface by combining simulations and experiments. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	2
35	Stability and molecular pathways to the formation of spin defects in silicon carbide. Nature Communications, 2021, 12, 6325.	12.8	9
36	Combined First-Principles Calculations of Electronâ€“Electron and Electronâ€“Phonon Self-Energies in Condensed Systems. Journal of Chemical Theory and Computation, 2021, 17, 7468-7476.	5.3	6

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37	Understanding the metal-to-insulator transition in La1â^'xSrxCoO3â^'Î´ and its applications for neuromorphic computing. Npj Computational Materials, 2020, 6, .	8.7	17
38	Can a PbCrO4 Photoanode Perform as Well as Isoelectronic BiVO4?. ACS Applied Energy Materials, 2020, 3, 8658-8666.	5.1	10
39	Stoichiometry of the Core Determines the Electronic Structure of Coreâ€“Shell IIIâ€“V/IIâ€“VI Nanoparticles. Chemistry of Materials, 2020, 32, 9798-9804.	6.7	14
40	Entanglement and control of single nuclear spins in isotopically engineered silicon carbide. Nature Materials, 2020, 19, 1319-1325.	27.5	98
41	First-principles studies of strongly correlated states in defect spin qubits in diamond. Physical Chemistry Chemical Physics, 2020, 22, 25522-25527.	2.8	22
42	PyCDFT : A Python package for constrained density functional theory. Journal of Computational Chemistry, 2020, 41, 1859-1867.	3.3	10
43	Dissociation of salts in water under pressure. Nature Communications, 2020, 11, 3037.	12.8	21
44	The Role of Surface Oxygen Vacancies in BiVO₄. Chemistry of Materials, 2020, 32, 2899-2909.	6.7	108
45	Molecular polarizabilities as fingerprints of perturbations to water by ions and confinement. Journal of Chemical Physics, 2020, 152, 124501.	3.0	11
46	Quantum simulations of materials on near-term quantum computers. Npj Computational Materials, 2020, 6, .	8.7	99
47	A first principles method to determine speciation of carbonates in supercritical water. Nature Communications, 2020, 11, 421.	12.8	21
48	Atomistic simulations of the thermal conductivity of liquids. Physical Review Materials, 2020, 4, .	2.4	9
49	Validating first-principles molecular dynamics calculations of oxide/water interfaces with x-ray reflectivity data. Physical Review Materials, 2020, 4, .	2.4	12
50	PyZFS: A Python package for first-principles calculations of zero-field splitting tensors. Journal of Open Source Software, 2020, 5, 2160.	4.6	10
51	Qresp, a tool for curating, discovering and exploring reproducible scientific papers. Scientific Data, 2019, 6, 190002.	5.3	24
52	Ab Initio Calculation of Equilibrium Isotopic Fractionations of Potassium and Rubidium in Minerals and Water. ACS Earth and Space Chemistry, 2019, 3, 2601-2612.	2.7	49
53	Modeling Superlattices of Dipolar and Polarizable Semiconducting Nanoparticles. Nano Letters, 2019, 19, 3912-3917.	9.1	6
54	Finite-Field Approach to Solving the Bethe-Salpeter Equation. Physical Review Letters, 2019, 122, 237402.	7.8	35

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55	Designing Janus Ligand Shells on PbS Quantum Dots using Ligandâ€“Ligand Cooperativity. ACS Nano, 2019, 13, 3839-3846.	14.6	23
56	Spin coherence in two-dimensional materials. Npj Computational Materials, 2019, 5, .	8.7	65
57	Spinâ€“phonon interactions in silicon carbide addressed by Gaussian acoustics. Nature Physics, 2019, 15, 490-495.	16.7	159
58	Improving the efficiency of G0W0 calculations with approximate spectral decompositions of dielectric matrices. Journal of Chemical Physics, 2019, 151, 224102.	3.0	6
59	A Finite-Field Approach for GW Calculations beyond the Random Phase Approximation. Journal of Chemical Theory and Computation, 2019, 15, 154-164.	5.3	21
60	All-electron density functional calculations for electron and nuclear spin interactions in molecules and solids. Physical Review Materials, 2019, 3, .	2.4	20
61	Dielectric-dependent hybrid functionals for heterogeneous materials. Physical Review Materials, 2019, 3, .	2.4	36
62	Computational prediction of lattice thermal conductivity: A comparison of molecular dynamics and Boltzmann transport approaches. Physical Review Materials, 2019, 3, .	2.4	29
63	Sterically controlled mechanochemistry under hydrostatic pressure. Nature, 2018, 554, 505-510.	27.8	71
64	Intra-molecular Charge Transfer and Electron Delocalization in Non-fullerene Organic Solar Cells. ACS Applied Materials & Interfaces, 2018, 10, 10043-10052.	8.0	24
65	Hierarchical Coupling of First-Principles Molecular Dynamics with Advanced Sampling Methods. Journal of Chemical Theory and Computation, 2018, 14, 2881-2888.	5.3	18
66	GW100: Comparison of Methods and Accuracy of Results Obtained with the WEST Code. Journal of Chemical Theory and Computation, 2018, 14, 1895-1909.	5.3	58
67	Electron affinity of liquid water. Nature Communications, 2018, 9, 247.	12.8	114
68	Excitations Partition into Two Distinct Populations in Bulk Perovskites. Advanced Optical Materials, 2018, 6, 1700975.	7.3	8
69	Emergent Electronic and Dielectric Properties of Interacting Nanoparticles at Finite Temperature. Nano Letters, 2018, 18, 255-261.	9.1	5
70	Optimizing materials for energy harvesting: in search for descriptors. , 2018, , .		0
71	Direct Synthesis of Six-Monolayer (1.9 nm) Thick Zinc-Blende CdSe Nanoplatelets Emitting at 585 nm. Chemistry of Materials, 2018, 30, 6957-6960.	6.7	77
72	Role of Point Defects in Enhancing the Conductivity of BiVO₄. Chemistry of Materials, 2018, 30, 7793-7802.	6.7	71

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73	Coupling First-Principles Calculations of Electronâ€“Electron and Electronâ€“Phonon Scattering, and Applications to Carbon-Based Nanostructures. Journal of Chemical Theory and Computation, 2018, 14, 6269-6275.	5.3	10
74	The role of defects and excess surface charges at finite temperature for optimizing oxide photoabsorbers. Nature Materials, 2018, 17, 1122-1127.	27.5	61
75	Enhanced Multiple Exciton Generation in PbS | CdS Janus-like Heterostructured Nanocrystals. ACS Nano, 2018, 12, 10084-10094.	14.6	56
76	First-Principles Simulations of Liquid Water Using a Dielectric-Dependent Hybrid Functional. Journal of Physical Chemistry Letters, 2018, 9, 3068-3073.	4.6	82
77	Optical Absorbance Enhancement in PbS QD/Cinnamate Ligand Complexes. Journal of Physical Chemistry Letters, 2018, 9, 3425-3433.	4.6	36
78	Surface chemistry and buried interfaces in all-inorganic nanocrystalline solids. Nature Nanotechnology, 2018, 13, 841-848.	31.5	30
79	Communication: Dielectric properties of condensed systems composed of fragments. Journal of Chemical Physics, 2018, 149, 051101.	3.0	9
80	Ab initio spectroscopy and ionic conductivity of water under Earth mantle conditions. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6952-6957.	7.1	34
81	Defect States and Charge Transport in Quantum Dot Solids. Chemistry of Materials, 2017, 29, 1255-1262.	6.7	33
82	Modelling heterogeneous interfaces for solar water splitting. Nature Materials, 2017, 16, 401-408.	27.5	252
83	Local and Global Effects of Dissolved Sodium Chloride on the Structure of Water. Journal of Physical Chemistry Letters, 2017, 8, 1496-1502.	4.6	87
84	Incorporation of Pyrazine and Bipyridine Linkers with High-Spin Fe(II) and Co(II) in a Metalâ€“Organic Framework. Inorganic Chemistry, 2017, 56, 3349-3356.	4.0	19
85	Characterization of NiFe oxyhydroxide electrocatalysts by integrated electronic structure calculations and spectroelectrochemistry. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3050-3055.	7.1	175
86	Charge Transport in Nanostructured Materials: Implementation and Verification of Constrained Density Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 2581-2590.	5.3	33
87	Tuning colloidal quantum dot band edge positions through solution-phase surface chemistry modification. Nature Communications, 2017, 8, 15257.	12.8	230
88	Performance and Self-Consistency of the Generalized Dielectric Dependent Hybrid Functional. Journal of Chemical Theory and Computation, 2017, 13, 3318-3325.	5.3	33
89	Design of Heterogeneous Chalcogenide Nanostructures with Pressure-Tunable Gaps and without Electronic Trap States. Nano Letters, 2017, 17, 2547-2553.	9.1	8
90	Instability and Efficiency of Mixed Halide Perovskites CH₃NH₃Al_{3â€“x}Cl_x (A = Pb and Sn): A First-Principles, Computational Study. Chemistry of Materials, 2017, 29, 682-689.	6.7	18

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91	Electronic structure of aqueous solutions: Bridging the gap between theory and experiments. Science Advances, 2017, 3, e1603210.	10.3	49
92	Hydrogen Treatment as a Detergent of Electronic Trap States in Lead Chalcogenide Nanoparticles. Chemistry of Materials, 2017, 29, 2485-2493.	6.7	14
93	Optimizing surface defects for atomic-scale electronics: Si dangling bonds. Physical Review Materials, 2017, 1, .	2.4	13
94	First-principles simulations of heat transport. Physical Review Materials, 2017, 1, .	2.4	35
95	Designing defect-based qubit candidates in wide-gap binary semiconductors for solid-state quantum technologies. Physical Review Materials, 2017, 1, .	2.4	43
96	Implementation and Validation of Fully Relativistic GW Calculations: Spinâ€“Orbit Coupling in Molecules, Nanocrystals, and Solids. Journal of Chemical Theory and Computation, 2016, 12, 3523-3544.	5.3	156
97	Blind test of density-functional-based methods on intermolecular interaction energies. Journal of Chemical Physics, 2016, 145, 124105.	3.0	97
98	Design of defect spins in piezoelectric aluminum nitride for solid-state hybrid quantum technologies. Scientific Reports, 2016, 6, 20803.	3.3	46
99	Novel silicon phases and nanostructures for solar energy conversion. Applied Physics Reviews, 2016, 3, .	11.3	68
100	Quantum decoherence dynamics of divacancy spins in silicon carbide. Nature Communications, 2016, 7, 12935.	12.8	128
101	Photoelectron Spectra of Aqueous Solutions from First Principles. Journal of the American Chemical Society, 2016, 138, 6912-6915.	13.7	64
102	Planarity and multiple components promote organic photovoltaic efficiency by improving electronic transport. Physical Chemistry Chemical Physics, 2016, 18, 31388-31399.	2.8	18
103	Nonempirical range-separated hybrid functionals for solids and molecules. Physical Review B, 2016, 93, .	3.2	125
104	The fate of carbon dioxide in water-rich fluids under extreme conditions. Science Advances, 2016, 2, e1601278.	10.3	50
105	Generalization of Dielectric-Dependent Hybrid Functionals to Finite Systems. Physical Review X, 2016, 6, .	8.9	49
106	Designing defect spins for wafer-scale quantum technologies. MRS Bulletin, 2015, 40, 1146-1153.	3.5	21
107	Colloidal nanoparticles for Intermediate Band solar cells. , 2015, , .		0
108	First-Principles Framework to Compute Sum-Frequency Generation Vibrational Spectra of Semiconductors and Insulators. Physical Review Letters, 2015, 115, 246404.	7.8	42

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109	Electronic Structure of IrO₂: The Role of the Metal d Orbitals. Journal of Physical Chemistry C, 2015, 119, 11570-11577.	3.1	91
110	Density and Compressibility of Liquid Water and Ice from First-Principles Simulations with Hybrid Functionals. Journal of Physical Chemistry Letters, 2015, 6, 2902-2908.	4.6	77
111	Large Scale GW Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2680-2696.	5.3	255
112	Tetrahedrally coordinated carbonates in Earthâ€™s lower mantle. Nature Communications, 2015, 6, 6311.	12.8	55
113	Electronic Energy Levels and Band Alignment for Aqueous Phenol and Phenolate from First Principles. Journal of Physical Chemistry B, 2015, 119, 9651-9660.	2.6	15
114	Colloidal Nanoparticles for Intermediate Band Solar Cells. ACS Nano, 2015, 9, 6882-6890.	14.6	37
115	The ionization potential of aqueous hydroxide computed using many-body perturbation theory. Journal of Chemical Physics, 2014, 141, 034501.	3.0	35
116	Probing the electronic structure of liquid water with many-body perturbation theory. Physical Review B, 2014, 89, .	3.2	61
117	Exotic phase Si nanoparticles and Si-ZnS nanocomposites: New paradigms to improve the efficiency of MEG solar cells. , 2014, , .		0
118	Dipolar correlations in liquid water. Journal of Chemical Physics, 2014, 141, 084504.	3.0	33
119	Si-based Earth abundant clathrates for solar energy conversion. Energy and Environmental Science, 2014, 7, 2598-2602.	30.8	31
120	Optimizing the Band Edges of Tungsten Trioxide for Water Oxidation: A First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 6019-6028.	3.1	63
121	Self-consistent hybrid functional for condensed systems. Physical Review B, 2014, 89, .	3.2	341
122	The refractive index and electronic gap of water and ice increase with increasing pressure. Nature Communications, 2014, 5, 3919.	12.8	70
123	Germanium nanoparticles with non-diamond core structures for solar energy conversion. Journal of Materials Chemistry A, 2014, 2, 9820.	10.3	29
124	Interfacial Effects on the Band Edges of Functionalized Si Surfaces in Liquid Water. Journal of the American Chemical Society, 2014, 136, 17071-17077.	13.7	81
125	Optoelectronic properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Ta</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:math>: A joint theoretical and experimental study. Physical Review B, 2014, 90, .	3.2	66
126	Electronic Structure of Aqueous Sulfuric Acid from First-Principles Simulations with Hybrid Functionals. Journal of Physical Chemistry Letters, 2014, 5, 2562-2567.	4.6	24

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127	Perovskites for Solar Thermoelectric Applications: A First Principle Study of CH₃NH₃Al₃ (A = Pb and Sn). Chemistry of Materials, 2014, 26, 5394-5400.	6.7	298
128	Solar Nanocomposites with Complementary Charge Extraction Pathways for Electrons and Holes: Si Embedded in ZnS. Physical Review Letters, 2014, 112, 106801.	7.8	22
129	Alumina(0001)/Water Interface: Structural Properties and Infrared Spectra from First-Principles Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2014, 118, 8944-8951.	3.1	47
130	Ab Initio Optoelectronic Properties of Silicon Nanoparticles: Excitation Energies, Sum Rules, and Tammâ€“Dancoff Approximation. Journal of Chemical Theory and Computation, 2014, 10, 3290-3298.	5.3	22
131	Structural and electronic properties of aqueous NaCl solutions from ab initio molecular dynamics simulations with hybrid density functionals. Chemical Physics Letters, 2014, 604, 89-96.	2.6	74
132	Strongly Anisotropic Dielectric Relaxation of Water at the Nanoscale. Journal of Physical Chemistry Letters, 2013, 4, 2477-2481.	4.6	104
133	Dielectric properties of water under extreme conditions and transport of carbonates in the deep Earth. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 6646-6650.	7.1	166
134	A closer look at supercritical water. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 6250-6251.	7.1	29
135	Dimensionality and heat transport in Si-Ge superlattices. Applied Physics Letters, 2013, 102, .	3.3	47
136	Spectral representation analysis of dielectric screening in solids and molecules. Physical Review B, 2013, 87, .	3.2	5
137	Electronic excitations in light absorbers for photoelectrochemical energy conversion: first principles calculations based on many body perturbation theory. Chemical Society Reviews, 2013, 42, 2437.	38.1	157
138	Increasing impact ionization rates in Si nanoparticles through surface engineering: A density functional study. Physical Review B, 2013, 87, .	3.2	24
139	Optical properties of tungsten trioxide from first-principles calculations. Physical Review B, 2013, 87, .	3.2	71
140	Communication: Electronic structure of the solvated chloride anion from first principles molecular dynamics. Journal of Chemical Physics, 2013, 138, 181102.	3.0	46
141	Band offsets and dielectric properties of the amorphous Si3N4/Si(100) interface: A first-principles study. Applied Physics Letters, 2013, 102, .	3.3	23
142	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>calculations using the spectral decomposition of the dielectric matrix: Verification, validation, and comparison of methods. Physical Review B, 2013, 87, .	3.2	120
143	Vibrational properties of alkyl monolayers on Si(111) surfaces: Predictions from ab-initio calculations. Applied Physics Letters, 2012, 100, 071605.	3.3	4
144	A Process for Visualizing Disordered Molecular Data with a Case Study in Bulk Water. , 2012, , .		1

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145	Improving accuracy and efficiency of calculations of photoemission spectra within the many-body perturbation theory. Physical Review B, 2012, 85, .	3.2	100
146	Tungsten Oxide Clathrates for Water Oxidation: A First Principles Study. Chemistry of Materials, 2012, 24, 4252-4260.	6.7	37
147	Probing the Structure of Salt Water under Confinement with First-Principles Molecular Dynamics and Theoretical X-ray Absorption Spectroscopy. Journal of Physical Chemistry Letters, 2012, 3, 2653-2658.	4.6	43
148	Solution of the Bethe-Salpeter equation without empty electronic states: Application to the absorption spectra of bulk systems. Physical Review B, 2012, 85, .	3.2	49
149	Structural and Vibrational Properties of Liquid Water from van der Waals Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 3054-3061.	5.3	146
150	First Principles Simulations of the Infrared Spectrum of Liquid Water Using Hybrid Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 1443-1449.	5.3	139
151	Heat transport in amorphous silicon: Interplay between morphology and disorder. Applied Physics Letters, 2011, 98, .	3.3	110
152	Microscopic modeling of the dielectric properties of silicon nitride. Physical Review B, 2011, 84, .	3.2	14
153	First-principles investigations of the dielectric properties of crystalline and amorphous Si3N4 thin films. Applied Physics Letters, 2010, 96, 062902.	3.3	25
154	Electronic and spectroscopic properties of the hydrogen-terminated Si(111) surface fromab initiocalculations. Physical Review B, 2010, 82, .	3.2	24
155	Ab initio calculations of optical absorption spectra: Solution of the Betheâ€“Salpeter equation within density matrix perturbation theory. Journal of Chemical Physics, 2010, 133, 164109.	3.0	132
156	Structural and Electronic Properties of the Methyl-Terminated Si(111) Surface. Journal of Physical Chemistry C, 2010, 114, 11898-11902.	3.1	14
157	Local Effects in the X-ray Absorption Spectrum of Salt Water. Journal of Physical Chemistry B, 2010, 114, 9594-9601.	2.6	41
158	First-Principle Analysis of the IR Stretching Band of Liquid Water. Journal of Physical Chemistry Letters, 2010, 1, 1398-1402.	4.6	45
159	First-principles study of electronic and vibrational properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BaHfN</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>Physical Review B, 2010, 82, .	3.2	26
160	Calculation of Quasi-Particle Energies of Aromatic Self-Assembled Monolayers on Au(111). Journal of Chemical Theory and Computation, 2009, 5, 881-886.	5.3	36
161	Iterative calculations of dielectric eigenvalue spectra. Physical Review B, 2009, 79, .	3.2	86
162	AbÂinitioCalculation of van der Waals Bonded Molecular Crystals. Physical Review Letters, 2009, 102, 206411.	7.8	133

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163	Practical algorithms to facilitate large-scale first-principles molecular dynamics. Journal of Physics: Conference Series, 2009, 180, 012074.	0.4	6
164	Water Confined in Nanotubes and between Graphene Sheets:â€‰ A First Principle Study. Journal of the American Chemical Society, 2008, 130, 1871-1878.	13.7	405
165	Dielectric Properties of Ice and Liquid Water from First-Principles Calculations. Physical Review Letters, 2008, 100, 147601.	7.8	63
166	Efficient iterative method for calculations of dielectric matrices. Physical Review B, 2008, 78, .	3.2	104
167	Melting of ice under pressure. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 14779-14783.	7.1	115
168	Role of dipolar correlations in the infrared spectra of water and ice. Physical Review B, 2008, 77, .	3.2	67
169	Dissecting hydrophobicity. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 2557-2558.	7.1	8
170	Electronic Properties of MoS₂ Nanoparticles. Journal of Physical Chemistry C, 2007, 111, 16192-16196.	3.1	634
171	Synthesis, Characterization, and Modeling of Nitrogen-Passivated Colloidal and Thin Film Silicon Nanocrystals. IEEE Journal of Selected Topics in Quantum Electronics, 2006, 12, 1151-1163.	2.9	13
172	Light-Emitting Silicon Nanocrystals and Photonic Structures in Silicon Nitride. IEEE Journal of Selected Topics in Quantum Electronics, 2006, 12, 1628-1635.	2.9	36
173	Water at a Hydrophilic Solid Surface Probed by Ab initio Molecular Dynamics:Â Inhomogeneous Thin Layers of Dense Fluid. Journal of the American Chemical Society, 2005, 127, 6830-6835.	13.7	64
174	Towards an assessment of the accuracy of density functional theory for first principles simulations of water. II. Journal of Chemical Physics, 2004, 121, 5400-5409.	3.0	338
175	Towards an assessment of the accuracy of density functional theory for first principles simulations of water. Journal of Chemical Physics, 2004, 120, 300-311.	3.0	489
176	Dissociation of Water under Pressure. Physical Review Letters, 2001, 87, 265501.	7.8	174
177	The solvation of Na+in water: First-principles simulations. Journal of Chemical Physics, 2000, 113, 4668-4673.	3.0	237
178	Twisted Aâ€Ðâ€A Type Acceptors with Thermallyâ€Activated Delayed Crystallization Behavior for Efficient Nonfullerene Organic Solar Cells. Advanced Energy Materials, 0, , 2103957.	19.5	6