Giulia Galli

List of Publications by Year
in descending order

178 papers	11,000 citations	25034 57 h-index	33894 99 g-index
182 all docs	182 docs citations	182 times ranked	12114 citing authors

#	Article	IF	Citations
1	Electronic Properties of MoS₂ Nanoparticles. Journal of Physical Chemistry C, 2007, 111, 16192-16196.	3.1	634
2	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
3	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
4	Self-consistent hybrid functional for condensed systems. Physical Review B, 2014, 89, .	3.2	341
5	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
6	Perovskites for Solar Thermoelectric Applications: A First Principle Study of CH₃NH₃AI₃ (A = Pb and Sn). Chemistry of Materials, 2014, 26, 5394-5400.	6.7	298
7	Large Scale GW Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2680-2696.	5.3	255
8	Modelling heterogeneous interfaces for solar water splitting. Nature Materials, 2017, 16, 401-408.	27.5	252
9	The solvation of Na+in water: First-principles simulations. Journal of Chemical Physics, 2000, 113, 4668-4673.	3.0	237
10	Tuning colloidal quantum dot band edge positions through solution-phase surface chemistry modification. Nature Communications, 2017, 8, 15257.	12.8	230
11	Quantum guidelines for solid-state spin defects. Nature Reviews Materials, 2021, 6, 906-925.	48.7	185
12	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
13	Dissociation of Water under Pressure. Physical Review Letters, 2001, 87, 265501.	7.8	174
14	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
15	Spinâ€“phonon interactions in silicon carbide addressed by Gaussian acoustics. Nature Physics, 2019, 15, 490-495.	16.7	159
16	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
17	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
18	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

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19	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
20	AbÂinitioCalculation of van der Waals Bonded Molecular Crystals. Physical Review Letters, 2009, 102, 206411.	7.8	133
21	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
22	Quantum decoherence dynamics of divacancy spins in silicon carbide. Nature Communications, 2016, 7, 12935.	12.8	128
23	Nonempirical range-separated hybrid functionals for solids and molecules. Physical Review B, 2016, 93, .	3.2	125
24	<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
25	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
26	Electron affinity of liquid water. Nature Communications, 2018, 9, 247.	12.8	114
27	Heat transport in amorphous silicon: Interplay between morphology and disorder. Applied Physics Letters, 2011, 98, .	3.3	110
28	The Role of Surface Oxygen Vacancies in BiVO₄. Chemistry of Materials, 2020, 32, 2899-2909.	6.7	108
29	The impact of surface composition on the interfacial energetics and photoelectrochemical properties of BiVO4. Nature Energy, 2021, 6, 287-294.	39.5	108
30	Efficient iterative method for calculations of dielectric matrices. Physical Review B, 2008, 78, .	3.2	104
31	Strongly Anisotropic Dielectric Relaxation of Water at the Nanoscale. Journal of Physical Chemistry Letters, 2013, 4, 2477-2481.	4.6	104
32	Improving accuracy and efficiency of calculations of photoemission spectra within the many-body perturbation theory. Physical Review B, 2012, 85, .	3.2	100
33	Quantum simulations of materials on near-term quantum computers. Npj Computational Materials, 2020, 6, .	8.7	99
34	Entanglement and control of single nuclear spins in isotopically engineered silicon carbide. Nature Materials, 2020, 19, 1319-1325.	27.5	98
35	Blind test of density-functional-based methods on intermolecular interaction energies. Journal of Chemical Physics, 2016, 145, 124105.	3.0	97
36	Electronic Structure of IrO₂: The Role of the Metal d Orbitals. Journal of Physical Chemistry C, 2015, 119, 11570-11577.	3.1	91

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37	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
38	Iterative calculations of dielectric eigenvalue spectra. Physical Review B, 2009, 79, .	3.2	86
39	First-Principles Simulations of Liquid Water Using a Dielectric-Dependent Hybrid Functional. Journal of Physical Chemistry Letters, 2018, 9, 3068-3073.	4.6	82
40	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
41	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
42	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
43	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
44	Optical properties of tungsten trioxide from first-principles calculations. Physical Review B, 2013, 87, .	3.2	71
45	Sterically controlled mechanochemistry under hydrostatic pressure. Nature, 2018, 554, 505-510.	27.8	71
46	Role of Point Defects in Enhancing the Conductivity of BiVO₄. Chemistry of Materials, 2018, 30, 7793-7802.	6.7	71
47	The refractive index and electronic gap of water and ice increase with increasing pressure. Nature Communications, 2014, 5, 3919.	12.8	70
48	Novel silicon phases and nanostructures for solar energy conversion. Applied Physics Reviews, 2016, 3, .	11.3	68
49	Role of dipolar correlations in the infrared spectra of water and ice. Physical Review B, 2008, 77, .	3.2	67
50	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
51	Spin coherence in two-dimensional materials. Npj Computational Materials, 2019, 5, .	8.7	65
52	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
53	Photoelectron Spectra of Aqueous Solutions from First Principles. Journal of the American Chemical Society, 2016, 138, 6912-6915.	13.7	64
54	Dielectric Properties of Ice and Liquid Water from First-Principles Calculations. Physical Review Letters, 2008, 100, 147601.	7.8	63

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55	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
56	Probing the electronic structure of liquid water with many-body perturbation theory. Physical Review B, 2014, 89, .	3.2	61
57	The role of defects and excess surface charges at finite temperature for optimizing oxide photoabsorbers. Nature Materials, 2018, 17, 1122-1127.	27.5	61
58	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
59	Five-second coherence of a single spin with single-shot readout in silicon carbide. Science Advances, 2022, 8, eabm5912.	10.3	57
60	Enhanced Multiple Exciton Generation in PbS | CdS Janus-like Heterostructured Nanocrystals. ACS Nano, 2018, 12, 10084-10094.	14.6	56
61	Tetrahedrally coordinated carbonates in Earthâ€™s lower mantle. Nature Communications, 2015, 6, 6311.	12.8	55
62	The fate of carbon dioxide in water-rich fluids under extreme conditions. Science Advances, 2016, 2, e1601278.	10.3	50
63	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
64	Generalization of Dielectric-Dependent Hybrid Functionals to Finite Systems. Physical Review X, 2016, 6, .	8.9	49
65	Electronic structure of aqueous solutions: Bridging the gap between theory and experiments. Science Advances, 2017, 3, e1603210.	10.3	49
66	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
67	Dimensionality and heat transport in Si-Ge superlattices. Applied Physics Letters, 2013, 102, .	3.3	47
68	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
69	Communication: Electronic structure of the solvated chloride anion from first principles molecular dynamics. Journal of Chemical Physics, 2013, 138, 181102.	3.0	46
70	Design of defect spins in piezoelectric aluminum nitride for solid-state hybrid quantum technologies. Scientific Reports, 2016, 6, 20803.	3.3	46
71	First-Principle Analysis of the IR Stretching Band of Liquid Water. Journal of Physical Chemistry Letters, 2010, 1, 1398-1402.	4.6	45
72	Quantum Embedding Theory for Strongly Correlated States in Materials. Journal of Chemical Theory and Computation, 2021, 17, 2116-2125.	5.3	45

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73	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
74	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
75	Designing defect-based qubit candidates in wide-gap binary semiconductors for solid-state quantum technologies. Physical Review Materials, 2017, 1, .	2.4	43
76	First-Principles Framework to Compute Sum-Frequency Generation Vibrational Spectra of Semiconductors and Insulators. Physical Review Letters, 2015, 115, 246404.	7.8	42
77	Integration of theory and experiment in the modelling of heterogeneous electrocatalysis. Nature Energy, 2021, 6, 700-705.	39.5	42
78	Local Effects in the X-ray Absorption Spectrum of Salt Water. Journal of Physical Chemistry B, 2010, 114, 9594-9601.	2.6	41
79	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
80	Tungsten Oxide Clathrates for Water Oxidation: A First Principles Study. Chemistry of Materials, 2012, 24, 4252-4260.	6.7	37
81	Colloidal Nanoparticles for Intermediate Band Solar Cells. ACS Nano, 2015, 9, 6882-6890.	14.6	37
82	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
83	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
84	Optical Absorbance Enhancement in PbS QD/Cinnamate Ligand Complexes. Journal of Physical Chemistry Letters, 2018, 9, 3425-3433.	4.6	36
85	Dielectric-dependent hybrid functionals for heterogeneous materials. Physical Review Materials, 2019, 3, .	2.4	36
86	The ionization potential of aqueous hydroxide computed using many-body perturbation theory. Journal of Chemical Physics, 2014, 141, 034501.	3.0	35
87	Finite-Field Approach to Solving the Bethe-Salpeter Equation. Physical Review Letters, 2019, 122, 237402.	7.8	35
88	First-principles simulations of heat transport. Physical Review Materials, 2017, 1, .	2.4	35
89	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
90	Dipolar correlations in liquid water. Journal of Chemical Physics, 2014, 141, 084504.	3.0	33

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91	Defect States and Charge Transport in Quantum Dot Solids. Chemistry of Materials, 2017, 29, 1255-1262.	6.7	33
92	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
93	Performance and Self-Consistency of the Generalized Dielectric Dependent Hybrid Functional. Journal of Chemical Theory and Computation, 2017, 13, 3318-3325.	5.3	33
94	Si-based Earth abundant clathrates for solar energy conversion. Energy and Environmental Science, 2014, 7, 2598-2602.	30.8	31
95	Surface chemistry and buried interfaces in all-inorganic nanocrystalline solids. Nature Nanotechnology, 2018, 13, 841-848.	31.5	30
96	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
97	Germanium nanoparticles with non-diamond core structures for solar energy conversion. Journal of Materials Chemistry A, 2014, 2, 9820.	10.3	29
98	Probing the Coherence of Solid-State Qubits at Avoided Crossings. PRX Quantum, 2021, 2, .	9.2	29
99	Photoluminescence spectra of point defects in semiconductors: Validation of first-principles calculations. Physical Review Materials, 2021, 5, .	2.4	29
100	Computational prediction of lattice thermal conductivity: A comparison of molecular dynamics and Boltzmann transport approaches. Physical Review Materials, 2019, 3, .	2.4	29
101	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
102	First-principles investigations of the dielectric properties of crystalline and amorphous Si3N4 thin films. Applied Physics Letters, 2010, 96, 062902.	3.3	25
103	Electronic and spectroscopic properties of the hydrogen-terminated Si(111) surface fromab initiocalculations. Physical Review B, 2010, 82, .	3.2	24
104	Increasing impact ionization rates in Si nanoparticles through surface engineering: A density functional study. Physical Review B, 2013, 87, .	3.2	24
105	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
106	Intra-molecular Charge Transfer and Electron Delocalization in Non-fullerene Organic Solar Cells. ACS Applied Materials & Interfaces, 2018, 10, 10043-10052.	8.0	24
107	Qresp, a tool for curating, discovering and exploring reproducible scientific papers. Scientific Data, 2019, 6, 190002.	5.3	24
108	Band offsets and dielectric properties of the amorphous Si3N4/Si(100) interface: A first-principles study. Applied Physics Letters, 2013, 102, .	3.3	23

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109	Designing Janus Ligand Shells on PbS Quantum Dots using Ligandâ€“Ligand Cooperativity. ACS Nano, 2019, 13, 3839-3846.	14.6	23
110	Solar Nanocomposites with Complementary Charge Extraction Pathways for Electrons and Holes: Si Embedded in ZnS. Physical Review Letters, 2014, 112, 106801.	7.8	22
111	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
112	First-principles studies of strongly correlated states in defect spin qubits in diamond. Physical Chemistry Chemical Physics, 2020, 22, 25522-25527.	2.8	22
113	Designing defect spins for wafer-scale quantum technologies. MRS Bulletin, 2015, 40, 1146-1153.	3.5	21
114	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
115	Dissociation of salts in water under pressure. Nature Communications, 2020, 11, 3037.	12.8	21
116	A first principles method to determine speciation of carbonates in supercritical water. Nature Communications, 2020, 11, 421.	12.8	21
117	All-electron density functional calculations for electron and nuclear spin interactions in molecules and solids. Physical Review Materials, 2019, 3, .	2.4	20
118	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
119	Planarity and multiple components promote organic photovoltaic efficiency by improving electronic transport. Physical Chemistry Chemical Physics, 2016, 18, 31388-31399.	2.8	18
120	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
121	Hierarchical Coupling of First-Principles Molecular Dynamics with Advanced Sampling Methods. Journal of Chemical Theory and Computation, 2018, 14, 2881-2888.	5.3	18
122	Simulating the Electronic Structure of Spin Defects on Quantum Computers. PRX Quantum, 2022, 3, .	9.2	18
123	Understanding the metal-to-insulator transition in La1â^'xSrxCoO3â^'Î´ and its applications for neuromorphic computing. Npj Computational Materials, 2020, 6, .	8.7	17
124	Greenâ€™s Function Formulation of Quantum Defect Embedding Theory. Journal of Chemical Theory and Computation, 2022, 18, 3512-3522.	5.3	17
125	Machine learning dielectric screening for the simulation of excited state properties of molecules and materials. Chemical Science, 2021, 12, 4970-4980.	7.4	16
126	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

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127	Structural and Electronic Properties of the Methyl-Terminated Si(111) Surface. Journal of Physical Chemistry C, 2010, 114, 11898-11902.	3.1	14
128	Microscopic modeling of the dielectric properties of silicon nitride. Physical Review B, 2011, 84, .	3.2	14
129	Hydrogen Treatment as a Detergent of Electronic Trap States in Lead Chalcogenide Nanoparticles. Chemistry of Materials, 2017, 29, 2485-2493.	6.7	14
130	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
131	PyCCE: A Python Package for Cluster Correlation Expansion Simulations of Spin Qubit Dynamics. Advanced Theory and Simulations, 2021, 4, 2100254.	2.8	14
132	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
133	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
134	Optimizing surface defects for atomic-scale electronics: Si dangling bonds. Physical Review Materials, 2017, 1, .	2.4	13
135	Spinâ€“spin interactions in defects in solids from mixed all-electron and pseudopotential first-principles calculations. Npj Computational Materials, 2021, 7, .	8.7	12
136	Quantum vibronic effects on the electronic properties of solid and molecular carbon. Physical Review Materials, 2021, 5, .	2.4	12
137	Observation of spatially resolved Rashba states on the surface of CH3NH3PbBr3 single crystals. Applied Physics Reviews, 2021, 8, .	11.3	12
138	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
139	Validating first-principles molecular dynamics calculations of oxide/water interfaces with x-ray reflectivity data. Physical Review Materials, 2020, 4, .	2.4	12
140	Molecular polarizabilities as fingerprints of perturbations to water by ions and confinement. Journal of Chemical Physics, 2020, 152, 124501.	3.0	11
141	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
142	Can a PbCrO4 Photoanode Perform as Well as Isoelectronic BiVO4?. ACS Applied Energy Materials, 2020, 3, 8658-8666.	5.1	10
143	PyCDFT : A Python package for constrained density functional theory. Journal of Computational Chemistry, 2020, 41, 1859-1867.	3.3	10
144	PyZFS: A Python package for first-principles calculations of zero-field splitting tensors. Journal of Open Source Software, 2020, 5, 2160.	4.6	10

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145	Communication: Dielectric properties of condensed systems composed of fragments. Journal of Chemical Physics, 2018, 149, 051101.	3.0	9
146	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
147	Substrate-controlled dynamics of spin qubits in low dimensional van der Waals materials. Applied Physics Letters, 2021, 118, .	3.3	9
148	Atomistic simulations of the thermal conductivity of liquids. Physical Review Materials, 2020, 4, .	2.4	9
149	Stability and molecular pathways to the formation of spin defects in silicon carbide. Nature Communications, 2021, 12, 6325.	12.8	9
150	Dissecting hydrophobicity. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 2557-2558.	7.1	8
151	Design of Heterogeneous Chalcogenide Nanostructures with Pressure-Tunable Gaps and without Electronic Trap States. Nano Letters, 2017, 17, 2547-2553.	9.1	8
152	Excitations Partition into Two Distinct Populations in Bulk Perovskites. Advanced Optical Materials, 2018, 6, 1700975.	7.3	8
153	Code interoperability extends the scope of quantum simulations. Npj Computational Materials, 2021, 7, .	8.7	8
154	Determining the Structureâ€“Property Relationships of Quasi-Two-Dimensional Semiconductor Nanoplatelets. Journal of Physical Chemistry C, 2021, 125, 4820-4827.	3.1	7
155	Cation and anion topotactic transformations in cobaltite thin films leading to Ruddlesden-Popper phases. Physical Review Materials, 2021, 5, .	2.4	7
156	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
157	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
158	Practical algorithms to facilitate large-scale first-principles molecular dynamics. Journal of Physics: Conference Series, 2009, 180, 012074.	0.4	6
159	Modeling Superlattices of Dipolar and Polarizable Semiconducting Nanoparticles. Nano Letters, 2019, 19, 3912-3917.	9.1	6
160	Improving the efficiency of G0W0 calculations with approximate spectral decompositions of dielectric matrices. Journal of Chemical Physics, 2019, 151, 224102.	3.0	6
161	Solvation of simple ions in water at extreme conditions. Journal of Chemical Physics, 2021, 154, 144501.	3.0	6
162	Theoretical and experimental study of the nitrogen-vacancy center in 4H-SiC. Physical Review Materials, 2021, 5, .	2.4	6

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163	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
164	Quantum simulations of thermally activated delayed fluorescence in an all-organic emitter. Physical Chemistry Chemical Physics, 2022, 24, 10101-10113.	2.8	6
165	Twisted Aâ€Dâ€A Type Acceptors with Thermallyâ€Activated Delayed Crystallization Behavior for Efficient Nonfullerene Organic Solar Cells. Advanced Energy Materials, 0, , 2103957.	19.5	6
166	Spectral representation analysis of dielectric screening in solids and molecules. Physical Review B, 2013, 87, .	3.2	5
167	Emergent Electronic and Dielectric Properties of Interacting Nanoparticles at Finite Temperature. Nano Letters, 2018, 18, 255-261.	9.1	5
168	Lessons learned from first-principles calculations of transition metal oxides. Journal of Chemical Physics, 2021, 154, 174704.	3.0	5
169	Vibrational properties of alkyl monolayers on Si(111) surfaces: Predictions from ab-initio calculations. Applied Physics Letters, 2012, 100, 071605.	3.3	4
170	Molecular Polarizabilities in Aqueous Systems from First-Principles. Journal of Physical Chemistry B, 2021, 125, 2183-2192.	2.6	4
171	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
172	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
173	Determining the Oxygen Stoichiometry of Cobaltite Thin Films. Chemistry of Materials, 2022, 34, 2076-2084.	6.7	2
174	A Process for Visualizing Disordered Molecular Data with a Case Study in Bulk Water. , 2012, , .		1
175	Photoelectron spectra of water and simple aqueous solutions at extreme conditions. Faraday Discussions, 2022, , .	3.2	1
176	Exotic phase Si nanoparticles and Si-ZnS nanocomposites: New paradigms to improve the efficiency of MEG solar cells. , 2014, , .		0
177	Colloidal nanoparticles for Intermediate Band solar cells. , 2015, , .		0
178	Optimizing materials for energy harvesting: in search for descriptors. , 2018, , .		0