Roberto Car

List of Publications by Year
in descending order

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202 papers	51,424 citations	7568 77 h-index	2178 202 g-index
204 all docs	204 docs citations	204 times ranked	46367 citing authors

#	Article	IF	Citations
1	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	1.8	18,183
2	Raman Spectra of Graphite Oxide and Functionalized Graphene Sheets. Nano Letters, 2008, 8, 36-41.	9.1	3,995
3	Single Sheet Functionalized Graphene by Oxidation and Thermal Expansion of Graphite. Chemistry of Materials, 2007, 19, 4396-4404.	6.7	3,276
4	Functionalized Single Graphene Sheets Derived from Splitting Graphite Oxide. Journal of Physical Chemistry B, 2006, 110, 8535-8539.	2.6	3,173
5	Car-Parrinello molecular dynamics with Vanderbilt ultrasoft pseudopotentials. Physical Review B, 1993, 47, 10142-10153.	3.2	1,303
6	Accurate and Efficient Method for Many-Body van der Waals Interactions. Physical Review Letters, 2012, 108, 236402.	7.8	1,120
7	Deep Potential Molecular Dynamics: A Scalable Model with the Accuracy of Quantum Mechanics. Physical Review Letters, 2018, 120, 143001.	7.8	1,006
8	Q<scp>uantum</scp> ESPRESSO toward the exascale. Journal of Chemical Physics, 2020, 152, 154105.	3.0	796
9	Oxygen-Driven Unzipping of Graphitic Materials. Physical Review Letters, 2006, 96, 176101.	7.8	524
10	Theory of Quantum Annealing of an Ising Spin Glass. Science, 2002, 295, 2427-2430.	12.6	489
11	Implementation of ultrasoft pseudopotentials inab initiomolecular dynamics. Physical Review B, 1991, 43, 6796-6799.	3.2	453
12	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.	1.1	445
13	Orbital formulation for electronic-structure calculations with linear system-size scaling. Physical Review B, 1993, 47, 9973-9976.	3.2	436
14	Metastable liquidâ€“liquid transition in a molecular model of water. Nature, 2014, 510, 385-388.	27.8	431
15	Two-Dimensional Self-Assembly of Supramolecular Clusters and Chains. Physical Review Letters, 1999, 83, 324-327.	7.8	396
16	Identification of Raman Defect Lines as Signatures of Ring Structures in Vitreous Silica. Physical Review Letters, 1998, 80, 5145-5147.	7.8	377
17	Nuclear Quantum Effects in Water. Physical Review Letters, 2008, 101, 017801.	7.8	361
18	First Solvation Shell of the Cu(II) Aqua Ion: Evidence for Fivefold Coordination. Science, 2001, 291, 856-859.	12.6	358

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19	Electronic and structural properties of sodium clusters. Physical Review B, 1985, 31, 1804-1816.	3.2	352
20	Ab initiomolecular dynamics ford-electron systems: Liquid copper at 1500 K. Physical Review Letters, 1992, 69, 1982-1985.	7.8	346
21	Ab initio theory and modeling of water. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10846-10851.	7.1	340
22	The role of vacancy defects and holes in the fracture of carbon nanotubes. Chemical Physics Letters, 2004, 390, 413-420.	2.6	338
23	Fully Unconstrained Approach to Noncollinear Magnetism: Application to Small Fe Clusters. Physical Review Letters, 1998, 80, 3622-3625.	7.8	331
24	Structural and Electronic Properties of Amorphous Carbon. Physical Review Letters, 1989, 62, 555-558.	7.8	301
25	Active learning of uniformly accurate interatomic potentials for materials simulation. Physical Review Materials, 2019, 3, .	2.4	299
26	Equilibrium Structures and Finite Temperature Properties of Silicon Microclusters fromab initioMolecular-Dynamics Calculations. Physical Review Letters, 1988, 60, 271-274.	7.8	279
27	The individual and collective effects of exact exchange and dispersion interactions on the ab initio structure of liquid water. Journal of Chemical Physics, 2014, 141, 084502.	3.0	276
28	Structural and Electronic Properties of Liquid and Amorphous SiO2: AnAb InitioMolecular Dynamics Study. Physical Review Letters, 1995, 74, 4682-4685.	7.8	266
29	Ab initiocalculation of properties of carbon in the amorphous and liquid states. Physical Review B, 1990, 42, 7470-7482.	3.2	258
30	Ab InitioMolecular Dynamics Study of First-Order Phase Transitions: Melting of Silicon. Physical Review Letters, 1995, 74, 1823-1826.	7.8	246
31	Interface structure between silicon and its oxide by first-principles molecular dynamics. Nature, 1998, 396, 58-60.	27.8	230
32	Generalized-gradient approximations to density-functional theory: A comparative study for atoms and solids. Physical Review B, 1996, 53, 1180-1185.	3.2	228
33	Theory of Si 2pcore-level shifts at the Si(001)-SiO2interface. Physical Review B, 1996, 53, 10942-10950.	3.2	211
34	Structure and Hyperfine Parameters ofE1â€²Centers inÎ±-Quartz and in VitreousSiO2. Physical Review Letters, 1997, 78, 887-890.	7.8	207
35	Carbon Phase Diagram fromAb InitioMolecular Dynamics. Physical Review Letters, 2005, 95, 185701.	7.8	206
36	Why Are Waterâ^'Hydrophobic Interfaces Charged?. Journal of the American Chemical Society, 2008, 130, 3915-3919.	13.7	204

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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.	7.8	193
38	Bending Properties of Single Functionalized Graphene Sheets Probed by Atomic Force Microscopy. ACS Nano, 2008, 2, 2577-2584.	14.6	187
39	Electronic properties of alkali trimers. Journal of Chemical Physics, 1983, 78, 5646-5655.	3.0	184
40	Model of vitreousSiO2generated by anab initiomolecular-dynamics quench from the melt. Physical Review B, 1995, 52, 12690-12695.	3.2	180
41	Si2pCore-Level Shifts at the Si(001)-SiO2Interface: A First-Principles Study. Physical Review Letters, 1995, 74, 1024-1027.	7.8	179
42	Hydroxide diffuses slower than hydronium in water because its solvated structure inhibits correlated proton transfer. Nature Chemistry, 2018, 10, 413-419.	13.6	175
43	Order-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>N</mml:mi></mml:math>implementation of exact exchange in extended insulating systems. Physical Review B, 2009, 79, .	3.2	171
44	Deep Potential: A General Representation of a Many-Body Potential Energy Surface. Communications in Computational Physics, 2018, 23, .	1.7	164
45	Dipolar Correlations and the Dielectric Permittivity of Water. Physical Review Letters, 2007, 98, 247401.	7.8	153
46	Calculation of near-edge x-ray-absorption fine structure at finite temperatures: Spectral signatures of hydrogen bond breaking in liquid water. Journal of Chemical Physics, 2004, 120, 8632-8637.	3.0	148
47	A comparison of methods for the calculation of NMR chemical shifts. Journal of Chemical Physics, 1999, 111, 1815-1822.	3.0	147
48	Microscopic Theory of Impurity-Defect Reactions and Impurity Diffusion in Silicon. Physical Review Letters, 1985, 54, 360-363.	7.8	146
49	Nitrogen Incorporation atSi(001)â^'SiO2Interfaces: Relation between N1sCore-Level Shifts and Microscopic Structure. Physical Review Letters, 1997, 79, 5174-5177.	7.8	142
50	First-principles molecular-dynamics study of the (0001)Î±â^'quartzsurface. Physical Review B, 2000, 61, 13250-13255.	3.2	142
51	Dynamical Charge Tensors and Infrared Spectrum of AmorphousSiO2. Physical Review Letters, 1997, 79, 1766-1769.	7.8	141
52	DeePCG: Constructing coarse-grained models via deep neural networks. Journal of Chemical Physics, 2018, 149, 034101.	3.0	141
53	Phase Diagram of a Deep Potential Water Model. Physical Review Letters, 2021, 126, 236001.	7.8	140
54	Combined Effects of Functional Groups, Lattice Defects, and Edges in the Infrared Spectra of Graphene Oxide. Journal of Physical Chemistry C, 2015, 119, 18167-18176.	3.1	134

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55	Free energy of proton transfer at the waterâ€“TiO₂ interface from ab initio deep potential molecular dynamics. Chemical Science, 2020, 11, 2335-2341.	7.4	134
56	Origin of the High-Frequency Doublet in the Vibrational Spectrum of Vitreous SiO2. Science, 1997, 275, 1925-1927.	12.6	133
57	Intermolecular Dynamical Charge Fluctuations in Water: A Signature of the H-Bond Network. Physical Review Letters, 2005, 95, 187401.	7.8	133
58	Reliable and practical computational description of molecular crystal polymorphs. Science Advances, 2019, 5, eaau3338.	10.3	127
59	Density Functional Theory of the Electrical Conductivity of Molecular Devices. Physical Review Letters, 2005, 94, 146803.	7.8	121
60	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.	3.0	119
61	A microscopic model for surface-induced diamond-to-graphite transitions. Nature, 1996, 379, 523-526.	27.8	115
62	Carbon: The nature of the liquid state. Physical Review Letters, 1989, 63, 988-991.	7.8	113
63	Signatures of a liquidâ€“liquid transition in an ab initio deep neural network model for water. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 26040-26046.	7.1	112
64	Structurally relaxed models of the Si(001)â€“SiO2 interface. Applied Physics Letters, 1996, 68, 625-627.	3.3	110
65	Electronic Structure and Reactivity of Isomeric Oxo-Mn(V) Porphyrins:Â Effects of Spin-State Crossing and pKaModulation. Inorganic Chemistry, 2006, 45, 4268-4276.	4.0	107
66	Dangling Bond Defects atSiâ^'SiO2Interfaces: Atomic Structure of thePb1Center. Physical Review Letters, 2000, 85, 2773-2776.	7.8	104
67	Simple, Unambiguous Theoretical Approach to Oxidation State Determination via First-Principles Calculations. Inorganic Chemistry, 2011, 50, 10259-10267.	4.0	103
68	Dynamic structure factor of vitreous silica from first principles: Comparison to neutron-inelastic-scattering experiments. Physical Review B, 1998, 57, 14133-14140.	3.2	100
69	86 PFLOPS Deep Potential Molecular Dynamics simulation of 100 million atoms with ab initio accuracy. Computer Physics Communications, 2021, 259, 107624.	7.5	100
70	Structure, growth, and bonding nature of Mg clusters. Physical Review B, 1991, 44, 8243-8255.	3.2	96
71	Local structure analysis in ab initio liquid water. Molecular Physics, 2015, 113, 2829-2841.	1.7	96
72	Structural and electronic properties of small copper clusters: a first principles study. Chemical Physics Letters, 1995, 238, 215-221.	2.6	91

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73	Pressure-Induced Structural Changes in LiquidSiO2fromAb InitioSimulations. Physical Review Letters, 2002, 89, 245504.	7.8	91
74	X-Ray Absorption Signatures of the Molecular Environment in Water and Ice. Physical Review Letters, 2010, 105, 017802.	7.8	85
75	The liquidâ€“liquid transition in supercooled ST2 water: a comparison between umbrella sampling and well-tempered metadynamics. Faraday Discussions, 2013, 167, 77.	3.2	85
76	Enhanced Thermal Decomposition of Nitromethane on Functionalized Graphene Sheets: Ab Initio Molecular Dynamics Simulations. Journal of the American Chemical Society, 2012, 134, 19011-19016.	13.7	83
77	Raman spectrum and polarizability of liquid water from deep neural networks. Physical Chemistry Chemical Physics, 2020, 22, 10592-10602.	2.8	80
78	Electronic Properties of Molecules and Surfaces with a Self-Consistent Interatomic van der Waals Density Functional. Physical Review Letters, 2015, 114, 176802.	7.8	79
79	Hydrophobic interaction and hydrogen-bond network for a methane pair in liquid water. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 2626-2630.	7.1	78
80	Short- and intermediate-range structure of liquid GeSe2. Physical Review B, 2001, 64, .	3.2	77
81	Equilibrium Geometries and Electronic Structures of Small Sodium Clusters. Physical Review Letters, 1984, 53, 655-658.	7.8	76
82	Microscopic Structure of LiquidGeSe2: The Problem of Concentration Fluctuations over Intermediate Range Distances. Physical Review Letters, 1998, 80, 2342-2345.	7.8	74
83	Interatomic potential for vanadium suitable for radiation damage simulations. Journal of Applied Physics, 2003, 93, 3328-3335.	2.5	74
84	Prediction of a magnetic Weyl semimetal without spin-orbit coupling and strong anomalous Hall effect in the Heusler compensated ferrimagnet <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ti</mml:mi><mml:mn>2</mml:mn></mml:m Physical Review B, 2018, 97, .	3.2	74
85	From Colossal to Zero: Controlling the Anomalous Hall Effect in Magnetic Heusler Compounds via Berry Curvature Design. Physical Review X, 2018, 8, .	8.9	74
86	Structure, Polarization, and Sum Frequency Generation Spectrum of Interfacial Water on Anatase TiO₂. Journal of Physical Chemistry Letters, 2018, 9, 6716-6721.	4.6	70
87	Pushing the Limit of Molecular Dynamics with Ab Initio Accuracy to 100 Million Atoms with Machine Learning. , 2020, , .		69
88	Ab initiostudy of positron trapping at a vacancy in GaAs. Physical Review Letters, 1994, 72, 3214-3217.	7.8	67
89	First-Principles Study of Excitonic Self-Trapping in Diamond. Physical Review Letters, 1995, 75, 3166-3169.	7.8	67
90	Role of dipolar correlations in the infrared spectra of water and ice. Physical Review B, 2008, 77, .	3.2	67

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91	First Principles Study of Photoelectron Spectra ofCunâ^'Clusters. Physical Review Letters, 1995, 75, 2104-2107.	7.8	66
92	Proton momentum distribution in water: an open path integral molecular dynamics study. Journal of Chemical Physics, 2007, 126, 234504.	3.0	66
93	Topological Nonsymmorphic Metals from Band Inversion. Physical Review X, 2016, 6, .	8.9	66
94	Tunneling and delocalization effects in hydrogen bonded systems: A study in position and momentum space. Journal of Chemical Physics, 2009, 130, 204511.	3.0	65
95	Current in Open Quantum Systems. Physical Review Letters, 2004, 93, 160404.	7.8	63
96	When do short-range atomistic machine-learning models fall short?. Journal of Chemical Physics, 2021, 154, 034111.	3.0	61
97	Energy-gap reduction in heavily doped silicon: Causes and consequences. Solid-State Electronics, 1985, 28, 17-24.	1.4	60
98	Tuning the Photoinduced O2-Evolving Reactivity of Mn4O47+, Mn4O46+, and Mn4O3(OH)6+ Manganeseâ^'Oxo Cubane Complexes. Inorganic Chemistry, 2006, 45, 189-195.	4.0	60
99	Deep neural network for the dielectric response of insulators. Physical Review B, 2020, 102, .	3.2	60
100	Intermediate Range Order and Bonding Character in Disordered Network-Forming Systems. Journal of the American Chemical Society, 1999, 121, 2943-2944.	13.7	59
101	Ab initio molecular dynamics with maximally localized Wannier functions. International Journal of Quantum Chemistry, 2003, 95, 821-829.	2.0	59
102	Fast algorithm for extracting the diagonal of the inverse matrix with application to the electronic structure analysis of metallic systems. Communications in Mathematical Sciences, 2009, 7, 755-777.	1.0	59
103	Comment on â€œThe putative liquid-liquid transition is a liquid-solid transition in atomistic models of waterâ€•[I and II: J. Chem. Phys. 135, 134503 (2011); J. Chem. Phys. 138, 214504 (2013)]. Journal of Chemical Physics, 2018, 148, 137101.	3.0	58
104	A deep potential model with long-range electrostatic interactions. Journal of Chemical Physics, 2022, 156, 124107.	3.0	57
105	The phase diagram of high-pressure superionic ice. Nature Communications, 2015, 6, 8156.	12.8	56
106	Diffusion mechanism of Cu adatoms on a Cu(001) surface. Surface Science, 1994, 306, L575-L578.	1.9	54
107	On the Mechanisms of OH Radical Induced DNA-Base Damage:Â A Comparative Quantum Chemical and Carâ^'Parrinello Molecular Dynamics Studyâ€. Journal of Physical Chemistry A, 2004, 108, 2922-2929.	2.5	54
108	Closing of the Nucleotide Pocket of Kinesin-Family Motors upon Binding to Microtubules. Science, 2003, 300, 798-801.	12.6	53

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109	Roles of quantum nuclei and inhomogeneous screening in the x-ray absorption spectra of water and ice. Physical Review B, 2012, 86, .	3.2	53
110	Isotope effects in liquid water via deep potential molecular dynamics. Molecular Physics, 2019, 117, 3269-3281.	1.7	52
111	Quantum Chemical Evaluation of Protein Control over Heme Ligation:Â CO/O2Discrimination in Myoglobin. Journal of Physical Chemistry B, 2005, 109, 3065-3070.	2.6	51
112	Large-Scale Structure and Hyperuniformity of Amorphous Ices. Physical Review Letters, 2017, 119, 136002.	7.8	50
113	Displaced Path Integral Formulation for the Momentum Distribution of Quantum Particles. Physical Review Letters, 2010, 105, 110602.	7.8	49
114	Influence of asymmetry on bias behavior of spin torque. Physical Review B, 2010, 81, .	3.2	47
115	Testing the TPSS meta-generalized-gradient-approximation exchange-correlation functional in calculations of transition states and reaction barriers. Journal of Chemical Physics, 2006, 125, 234104.	3.0	46
116	Correlated Tunneling in Hydrogen Bonds. Journal of Statistical Physics, 2011, 145, 365-384.	1.2	45
117	Use of dielectric functions in the theory of dispersion forces. Physical Review B, 2005, 71, .	3.2	44
118	Hybrid density functional calculations of the band gap of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ga</mml:mtext></mml:mrow><mml:mi>x</mml:mi></mml:msub> Physical Review B, 2009, 80, .	3.2	41
119	Local-order metric for condensed-phase environments. Physical Review B, 2018, 97, .	3.2	41
120	SpherosiloxaneH8Si8O12clusters on Si(001): First-principles calculation of Si2pcore-level shifts. Physical Review B, 1996, 54, R2339-R2342.	3.2	38
121	Role of Ligand Bending in the Photodissociation of O2vs CO-heme:Â A Time-Dependent Density Functional Study. Journal of the American Chemical Society, 2003, 125, 15710-15711.	13.7	38
122	Fixing Jacob's ladder. Nature Chemistry, 2016, 8, 820-821.	13.6	37
123	Assessment of the Tao-Mo nonempirical semilocal density functional in applications to solids and surfaces. Physical Review B, 2017, 95, .	3.2	37
124	Phase Equilibrium of Water with Hexagonal and Cubic Ice Using the SCAN Functional. Journal of Chemical Theory and Computation, 2021, 17, 3065-3077.	5.3	37
125	Searching for crystal-ice domains in amorphous ices. Physical Review Materials, 2018, 2, .	2.4	37
126	A Classical and Ab Initio Study of the Interaction of the Myosin Triphosphate Binding Domain with ATP. Biophysical Journal, 2002, 82, 660-675.	0.5	35

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127	Anisotropic Adsorption of Molecular Assemblies on Crystalline Surfaces. Journal of Physical Chemistry B, 2006, 110, 16624-16632.	2.6	34
128	Quantization of the dipole moment and of the end charges in push-pull polymers. Journal of Chemical Physics, 2007, 127, 194902.	3.0	34
129	Theory of electronically stimulated defect migration in semiconductors. Physical Review B, 1984, 30, 2260-2262.	3.2	33
130	Dynamics of structural relaxation upon Rydberg excitation of an impurity in an Ar crystal. Chemical Physics, 1998, 233, 343-352.	1.9	33
131	Chemistry between Magnesium and Multiple Molecules in Tris(8-hydroxyquinoline) Aluminum Films. Journal of the American Chemical Society, 2003, 125, 7808-7809.	13.7	33
132	Band alignment in molecular devices: Influence of anchoring group and metal work function. Physical Review B, 2008, 77, .	3.2	33
133	Simulation of Electrocatalytic Hydrogen Production by a Bioinspired Catalyst Anchored to a Pyrite Electrode. Journal of the American Chemical Society, 2010, 132, 8593-8601.	13.7	33
134	Momentum distribution, vibrational dynamics, and the potential of mean force in ice. Physical Review B, 2011, 83, .	3.2	33
135	Analytical nuclear gradients for the range-separated many-body dispersion model of noncovalent interactions. Chemical Science, 2016, 7, 1712-1728.	7.4	33
136	Auxiliary-field quantum Monte Carlo calculations for systems with long-range repulsive interactions. Physical Review Letters, 1993, 71, 1148-1151.	7.8	32
137	Reconstruction of frozen-core all-electron orbitals from pseudo-orbitals. Journal of Chemical Physics, 2001, 115, 5791-5795.	3.0	32
138	Band Engineering of Dirac Semimetals Using Charge Density Waves. Advanced Materials, 2021, 33, e2101591.	21.0	32
139	Role of Molecular Conjugation in the Surface Radical Reaction of Aldehydes with Hâ^'Si(111):â€‰ First Principles Study. Journal of Physical Chemistry B, 2005, 109, 18889-18894.	2.6	31
140	Oxidation State Changes and Electron Flow in Enzymatic Catalysis and Electrocatalysis through Wannierâ€Function Analysis. Chemistry - A European Journal, 2011, 17, 12136-12143.	3.3	30
141	Resolving the CO/CN Ligand Arrangement in CO-Inactivated [FeFe] Hydrogenase by First Principles Density Functional Theory Calculations. Inorganic Chemistry, 2006, 45, 5715-5717.	4.0	29
142	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.	5.3	29
143	Heat transport in liquid water from first-principles and deep neural network simulations. Physical Review B, 2021, 104, .	3.2	29
144	Berry phase approach to longitudinal dipole moments of infinite chains in electronic-structure methods with local basis sets. Journal of Chemical Physics, 2007, 126, 234101.	3.0	27

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145	Interpretation of photoelectron spectra inCunâ^'clusters including thermal and final-state effects: The case ofCu7â^'. Physical Review B, 1996, 54, 8913-8918.	3.2	26
146	Self-interstitial transport in vanadium. Acta Materialia, 2005, 53, 1985-1994.	7.9	26
147	First-principles electronic structure study of Ti-PTCDA contacts. Physical Review B, 2002, 65, .	3.2	25
148	Theoretical Studies of [FeFe]-Hydrogenase:Â Structure and Infrared Spectra of Synthetic Models. Journal of Physical Chemistry B, 2006, 110, 7049-7057.	2.6	25
149	Performance of a nonempirical density functional on molecules and hydrogen-bonded complexes. Journal of Chemical Physics, 2016, 145, 234306.	3.0	25
150	Mapping potential energy surfaces. Journal of Chemical Physics, 2004, 121, 1193-1200.	3.0	23
151	Viscosity in water from first-principles and deep-neural-network simulations. Npj Computational Materials, 2022, 8, .	8.7	23
152	Tunneling Conductance of Amine-Linked Alkyl Chains. Nano Letters, 2008, 8, 1771-1777.	9.1	22
153	In situ Characterization of Nanoparticles Using Rayleigh Scattering. Scientific Reports, 2017, 7, 40230.	3.3	22
154	Longitudinal polarizability of long polymeric chains: Quasi-one-dimensional electrostatics as the origin of slow convergence. Journal of Chemical Physics, 2005, 122, 134907.	3.0	21
155	A Theoretical Study of Biotin Chemisorption on Siâ^'SiC(001) Surfaces. Journal of Physical Chemistry B, 2005, 109, 13656-13662.	2.6	20
156	Root-growth of boron nitride nanotubes: experiments and ab initio simulations. Nanoscale, 2018, 10, 22223-22230.	5.6	19
157	Structure and electronic properties of amorphous indium phosphide from first principles. Physical Review B, 1998, 57, 1594-1606.	3.2	18
158	Thermal expansion in dispersion-bound molecular crystals. Physical Review Materials, 2018, 2, .	2.4	18
159	Cu++ and Li+ interaction with polyethylene oxide byab initiomolecular dynamics. Journal of Chemical Physics, 1998, 108, 9933-9936.	3.0	17
160	Palmer et al. reply. Nature, 2016, 531, E2-E3.	27.8	17
161	First-principles free-energy calculations on condensed-matter systems: Lattice vacancy in silicon. Physical Review B, 1996, 53, 9760-9763.	3.2	16
162	Minimization of the potential energy surface of Lennardâ€"Jones clusters by quantum optimization. Chemical Physics Letters, 2005, 412, 125-130.	2.6	16

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163	Concentration fluctuations on intermediate range distances in liquid GeSe2: the critical role of ionicity. Computational Materials Science, 2000, 17, 115-121.	3.0	15
164	Structures, Interactions, and Ferromagnetism of Feâ^'Carbon Nanotube Systems. Journal of Physical Chemistry C, 2008, 112, 8400-8407.	3.1	15
165	Phase equilibrium of liquid water and hexagonal ice from enhanced sampling molecular dynamics simulations. Journal of Chemical Physics, 2020, 152, 204116.	3.0	15
166	Theoretical Design by First Principles Molecular Dynamics of a Bioinspired Electrodeâ^'Catalyst System for Electrocatalytic Hydrogen Production from Acidified Water. Journal of Chemical Theory and Computation, 2010, 6, 3490-3502.	5.3	14
167	Designer spin systems via inverse statistical mechanics. Physical Review B, 2013, 88, .	3.2	14
168	Inverse design of disordered stealthy hyperuniform spin chains. Physical Review B, 2016, 93, .	3.2	14
169	Manifestations of metastable criticality in the long-range structure of model water glasses. Nature Communications, 2021, 12, 3398.	12.8	14
170	Influence of point defects on the electronic and topological properties of monolayer <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></mml Physical Review B, 2020, 102, .	3.2	14
171	Theoretical Studies of [FeFe]-Hydrogenase:Â Infrared Fingerprints of the Dithiol-Bridging Ligand in the Active Site. Inorganic Chemistry, 2007, 46, 1153-1161.	4.0	13
172	Charge Transfer in Partition Theory. Journal of Physical Chemistry A, 2009, 113, 2183-2192.	2.5	13
173	Mechanism of H₂ Production by the [FeFe]_H Subcluster of Di-Iron Hydrogenases: Implications for Abiotic Catalysts. Journal of Physical Chemistry B, 2008, 112, 13381-13390.	2.6	12
174	Theory of tunneling transport in periodic chains. Physical Review B, 2009, 80, .	3.2	12
175	A well-scaling natural orbital theory. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 12913-12918.	7.1	11
176	Migration of a carbon adatom on a charged single-walled carbon nanotube. Carbon, 2017, 116, 174-180.	10.3	11
177	Variational Approach to MonteÂCarlo Renormalization Group. Physical Review Letters, 2017, 119, 220602.	7.8	11
178	Hydrogen Dynamics in Supercritical Water Probed by Neutron Scattering and Computer Simulations. Journal of Physical Chemistry Letters, 2020, 11, 9461-9467.	4.6	11
179	Many-body effects in the X-ray absorption spectra of liquid water. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2201258119.	7.1	11
180	Free energy profile along a discretized reaction path via the hyperplane constraint force and torque. Journal of Chemical Physics, 2005, 122, 114108.	3.0	10

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181	Hydrogen Production by the Naked Active Site of the Di-iron Hydrogenases in Water. Journal of Physical Chemistry B, 2009, 113, 13096-13106.	2.6	10
182	Forces in pseudopotential molecular calculations. Journal of Chemical Physics, 1984, 80, 1525-1528.	3.0	8
183	Low- and high-temperature phases of a Pb monolayer on Ge(111) fromab initiomolecular dynamics. Physical Review B, 1994, 50, 15158-15165.	3.2	8
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