Roberto Car

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/116405/publications.pdf

Version: 2024-02-01

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	A deep potential model with long-range electrostatic interactions. Journal of Chemical Physics, 2022, 156, 124107.	3.0	57
2	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
3	Phase diagram of the TIP4P/Ice water model by enhanced sampling simulations. Journal of Chemical Physics, 2022, 157, .	3.0	8
4	Viscosity in water from first-principles and deep-neural-network simulations. Npj Computational Materials, 2022, 8, .	8.7	23
5	86 PFLOPS Deep Potential Molecular Dynamics simulation of 100 million atoms with ab initio accuracy. Computer Physics Communications, 2021, 259, 107624.	7.5	100
6	When do short-range atomistic machine-learning models fall short?. Journal of Chemical Physics, 2021, 154, 034111.	3.0	61
7	Enhancing the formation of ionic defects to study the ice Ih/XI transition with molecular dynamics simulations. Molecular Physics, 2021, 119, .	1.7	7
8	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
9	Band Engineering of Dirac Semimetals Using Charge Density Waves. Advanced Materials, 2021, 33, e2101591.	21.0	32
10	Phase Diagram of a Deep Potential Water Model. Physical Review Letters, 2021, 126, 236001.	7.8	140
11	Manifestations of metastable criticality in the long-range structure of model water glasses. Nature Communications, 2021, 12, 3398.	12.8	14
12	Heat transport in liquid water from first-principles and deep neural network simulations. Physical Review B, 2021, 104, .	3.2	29
13	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
14	Deep neural network for the dielectric response of insulators. Physical Review B, 2020, 102, .	3.2	60
15	Continuous-time Monte Carlo renormalization group. Physical Review B, 2020, 102, .	3.2	3
16	Hydrogen Dynamics in Supercritical Water Probed by Neutron Scattering and Computer Simulations. Journal of Physical Chemistry Letters, 2020, 11, 9461-9467.	4.6	11
17	MonteÂCarlo Renormalization Group for Classical Lattice Models with Quenched Disorder. Physical Review Letters, 2020, 125, 190601.	7.8	1
18	Raman spectrum and polarizability of liquid water from deep neural networks. Physical Chemistry Chemical Physics, 2020, 22, 10592-10602.	2.8	80

#	Article	IF	Citations
19	Phase equilibrium of liquid water and hexagonal ice from enhanced sampling molecular dynamics simulations. Journal of Chemical Physics, 2020, 152, 204116.	3.0	15
20	Quantum momentum distribution and quantum entanglement in the deep tunneling regime. Journal of Chemical Physics, 2020, 152, 024106.	3.0	1
21	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
22	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
23	Q<scp>uantum</scp> ESPRESSO toward the exascale. Journal of Chemical Physics, 2020, 152, 154105.	3.0	796
24	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:math> Physical Review B, 2020, 102, .	3.2	14
25	Pushing the Limit of Molecular Dynamics with Ab Initio Accuracy to 100 Million Atoms with Machine Learning. , 2020, , .		69
26	Isotope effects in liquid water via deep potential molecular dynamics. Molecular Physics, 2019, 117, 3269-3281.	1.7	52
27	Determination of the critical manifold tangent space and curvature with Monte Carlo renormalization group. Physical Review E, 2019, 100, 022138.	2.1	4
28	Reliable and practical computational description of molecular crystal polymorphs. Science Advances, 2019, 5, eaau3338.	10.3	127
29	Active learning of uniformly accurate interatomic potentials for materials simulation. Physical Review Materials, 2019, 3, .	2.4	299
30	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
31	Deep Potential Molecular Dynamics: A Scalable Model with the Accuracy of Quantum Mechanics. Physical Review Letters, 2018, 120, 143001.	7.8	1,006
32	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
33	Local-order metric for condensed-phase environments. Physical Review B, 2018, 97, .	3.2	41
34	Hydroxide diffuses slower than hydronium in water because its solvated structure inhibits correlated proton transfer. Nature Chemistry, 2018, 10, 413-419.	13.6	175
35	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
36	Occupation probabilities as variables in electronic structure theory: cooper pairing, OP-NSOFT-Cs,t, and the homogeneous electron liquid. European Physical Journal B, 2018, 91, 1.	1.5	1

#	Article	IF	Citations
37	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
38	Root-growth of boron nitride nanotubes: experiments and ab initio simulations. Nanoscale, 2018, 10, 22223-22230.	5.6	19
39	DeePCG: Constructing coarse-grained models via deep neural networks. Journal of Chemical Physics, 2018, 149, 034101.	3.0	141
40	Thermal expansion in dispersion-bound molecular crystals. Physical Review Materials, 2018, 2, .	2.4	18
41	Searching for crystal-ice domains in amorphous ices. Physical Review Materials, 2018, 2, .	2.4	37
42	Deep Potential: A General Representation of a Many-Body Potential Energy Surface. Communications in Computational Physics, 2018, 23, .	1.7	164
43	In situ Characterization of Nanoparticles Using Rayleigh Scattering. Scientific Reports, 2017, 7, 40230.	3.3	22
44	Assessment of the Tao-Mo nonempirical semilocal density functional in applications to solids and surfaces. Physical Review B, 2017, 95, .	3.2	37
45	Migration of a carbon adatom on a charged single-walled carbon nanotube. Carbon, 2017, 116, 174-180.	10.3	11
46	Large-Scale Structure and Hyperuniformity of Amorphous Ices. Physical Review Letters, 2017, 119, 136002.	7.8	50
47	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
48	Variational Approach to MonteÂCarlo Renormalization Group. Physical Review Letters, 2017, 119, 220602.	7.8	11
49	Topological Nonsymmorphic Metals from Band Inversion. Physical Review X, 2016, 6, .	8.9	66
50	Performance of a nonempirical density functional on molecules and hydrogen-bonded complexes. Journal of Chemical Physics, 2016, 145, 234306.	3.0	25
51	Fixing Jacob's ladder. Nature Chemistry, 2016, 8, 820-821.	13.6	37
52	Fermionic Symmetry-Protected Topological Phase in a Two-Dimensional Hubbard Model. Physical Review Letters, 2016, 117, 096405.	7.8	7
53	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
54	Inverse design of disordered stealthy hyperuniform spin chains. Physical Review B, 2016, 93, .	3.2	14

#	Article	IF	Citations
55	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
56	Palmer et al. reply. Nature, 2016, 531, E2-E3.	27.8	17
57	Analytical nuclear gradients for the range-separated many-body dispersion model of noncovalent interactions. Chemical Science, 2016, 7, 1712-1728.	7.4	33
58	Local structure analysis in ab initio liquid water. Molecular Physics, 2015, 113, 2829-2841.	1.7	96
59	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
60	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
61	The phase diagram of high-pressure superionic ice. Nature Communications, 2015, 6, 8156.	12.8	56
62	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
63	MÃ¶bius molecules and fragile Mott insulators. Physical Review B, 2014, 90, .	3.2	3
64	Metastable liquidâ€“liquid transition in a molecular model of water. Nature, 2014, 510, 385-388.	27.8	431
65	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
66	Oxygen tolerance of an in silico -designed bioinspired hydrogen-evolving catalyst in water. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 2017-2022.	7.1	6
67	Designer spin systems via inverse statistical mechanics. Physical Review B, 2013, 88, .	3.2	14
68	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
69	PHONON-INDUCED ANISOTROPIC DISPERSION FORCES ON A METALLIC SUBSTRATE. Nano LIFE, 2012, 02, 1240001.	0.9	2
70	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
71	Accurate and Efficient Method for Many-Body van der Waals Interactions. Physical Review Letters, 2012, 108, 236402.	7.8	1,120
72	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

#	Article	IF	Citations
73	Hydrogen Bonds and van der Waals Forces in Ice at Ambient and High Pressures. Physical Review Letters, 2011, 107, 185701.	7.8	193
74	Simple, Unambiguous Theoretical Approach to Oxidation State Determination via First-Principles Calculations. Inorganic Chemistry, 2011, 50, 10259-10267.	4.0	103
75	Correlated Tunneling in Hydrogen Bonds. Journal of Statistical Physics, 2011, 145, 365-384.	1.2	45
76	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
77	Electrocatalyst design from first principles: A hydrogen-production catalyst inspired by nature. Catalysis Today, 2011, 165, 160-170.	4.4	6
78	Effect of disorder on spin-transfer torque in magnetic tunnel junctions. Journal of Applied Physics, 2011, 109, 07C920.	2.5	4
79	Momentum distribution, vibrational dynamics, and the potential of mean force in ice. Physical Review B, 2011, 83, .	3.2	33
80	Displaced Path Integral Formulation for the Momentum Distribution of Quantum Particles. Physical Review Letters, 2010, 105, 110602.	7.8	49
81	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
82	X-Ray Absorption Signatures of the Molecular Environment in Water and Ice. Physical Review Letters, 2010, 105, 017802.	7.8	85
83	Influence of asymmetry on bias behavior of spin torque. Physical Review B, 2010, 81, .	3.2	47
84	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
85	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
86	Theory of tunneling transport in periodic chains. Physical Review B, 2009, 80, .	3.2	12
87	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
88	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
89	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
90	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

#	Article	IF	Citations
91	Charge Transfer in Partition Theory. Journal of Physical Chemistry A, 2009, 113, 2183-2192.	2.5	13
92	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
93	Raman Spectra of Graphite Oxide and Functionalized Graphene Sheets. Nano Letters, 2008, 8, 36-41.	9.1	3,995
94	Why Are Waterâ^'Hydrophobic Interfaces Charged?. Journal of the American Chemical Society, 2008, 130, 3915-3919.	13.7	204
95	Bending Properties of Single Functionalized Graphene Sheets Probed by Atomic Force Microscopy. ACS Nano, 2008, 2, 2577-2584.	14.6	187
96	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
97	Structures, Interactions, and Ferromagnetism of Feâ^'Carbon Nanotube Systems. Journal of Physical Chemistry C, 2008, 112, 8400-8407.	3.1	15
98	Dynamical Optimization for Partition Theory. Journal of Physical Chemistry A, 2008, 112, 571-575.	2.5	2
99	Tunneling Conductance of Amine-Linked Alkyl Chains. Nano Letters, 2008, 8, 1771-1777.	9.1	22
100	Role of dipolar correlations in the infrared spectra of water and ice. Physical Review B, 2008, 77, .	3.2	67
101	Band alignment in molecular devices: Influence of anchoring group and metal work function. Physical Review B, 2008, 77, .	3.2	33
102	Nuclear Quantum Effects in Water. Physical Review Letters, 2008, 101, 017801.	7.8	361
103	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
104	Quantization of the dipole moment and of the end charges in push-pull polymers. Journal of Chemical Physics, 2007, 127, 194902.	3.0	34
105	Proton momentum distribution in water: an open path integral molecular dynamics study. Journal of Chemical Physics, 2007, 126, 234504.	3.0	66
106	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
107	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
108	Dipolar Correlations and the Dielectric Permittivity of Water. Physical Review Letters, 2007, 98, 247401.	7.8	153

#	Article	IF	Citations
109	Single Sheet Functionalized Graphene by Oxidation and Thermal Expansion of Graphite. Chemistry of Materials, 2007, 19, 4396-4404.	6.7	3,276
110	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
111	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
112	Anisotropic Adsorption of Molecular Assemblies on Crystalline Surfaces. Journal of Physical Chemistry B, 2006, 110, 16624-16632.	2.6	34
113	Oxygen-Driven Unzipping of Graphitic Materials. Physical Review Letters, 2006, 96, 176101.	7.8	524
114	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
115	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
116	Orbital Energetics and Molecular Recognition. Journal of the American Chemical Society, 2006, 128, 4514-4515.	13.7	1
117	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
118	Functionalized Single Graphene Sheets Derived from Splitting Graphite Oxide. Journal of Physical Chemistry B, 2006, 110, 8535-8539.	2.6	3,173
119	Self-interstitial transport in vanadium. Acta Materialia, 2005, 53, 1985-1994.	7.9	26
120	Minimization of the potential energy surface of Lennardâ€"Jones clusters by quantum optimization. Chemical Physics Letters, 2005, 412, 125-130.	2.6	16
121	Carbon Phase Diagram fromAb InitioMolecular Dynamics. Physical Review Letters, 2005, 95, 185701.	7.8	206
122	Electron transport with dissipation: A quantum kinetic approach. International Journal of Quantum Chemistry, 2005, 101, 564-571.	2.0	7
123	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
124	Density Functional Theory of the Electrical Conductivity of Molecular Devices. Physical Review Letters, 2005, 94, 146803.	7.8	121
125	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
126	Use of dielectric functions in the theory of dispersion forces. Physical Review B, 2005, 71, .	3.2	44

#	Article	IF	Citations
127	Intermolecular Dynamical Charge Fluctuations in Water: A Signature of the H-Bond Network. Physical Review Letters, 2005, 95, 187401.	7.8	133
128	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
129	A Theoretical Study of Biotin Chemisorption on Siâˆ’SiC(001) Surfaces. Journal of Physical Chemistry B, 2005, 109, 13656-13662.	2.6	20
130	Role of Molecular Conjugation in the Surface Radical Reaction of Aldehydes with Hâˆ’Si(111):â€‰ First Principles Study. Journal of Physical Chemistry B, 2005, 109, 18889-18894.	2.6	31
131	Mapping potential energy surfaces. Journal of Chemical Physics, 2004, 121, 1193-1200.	3.0	23
132	Current in Open Quantum Systems. Physical Review Letters, 2004, 93, 160404.	7.8	63
133	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
134	The role of vacancy defects and holes in the fracture of carbon nanotubes. Chemical Physics Letters, 2004, 390, 413-420.	2.6	338
135	On the Mechanisms of OH Radical Induced DNA-Base Damage:Â A Comparative Quantum Chemical and Carâˆ’Parrinello Molecular Dynamics Studyâ€. Journal of Physical Chemistry A, 2004, 108, 2922-2929.	2.5	54
136	Ab initio molecular dynamics with maximally localized Wannier functions. International Journal of Quantum Chemistry, 2003, 95, 821-829.	2.0	59
137	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
138	Interatomic potential for vanadium suitable for radiation damage simulations. Journal of Applied Physics, 2003, 93, 3328-3335.	2.5	74
139	Closing of the Nucleotide Pocket of Kinesin-Family Motors upon Binding to Microtubules. Science, 2003, 300, 798-801.	12.6	53
140	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
141	First-principles electronic structure study of Ti-PTCDA contacts. Physical Review B, 2002, 65, .	3.2	25
142	Pressure-Induced Structural Changes in LiquidSiO2fromAb InitioSimulations. Physical Review Letters, 2002, 89, 245504.	7.8	91
143	Theory of Quantum Annealing of an Ising Spin Glass. Science, 2002, 295, 2427-2430.	12.6	489
144	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

#	Article	IF	Citations
145	First Solvation Shell of the Cu(II) Aqua Ion: Evidence for Fivefold Coordination. Science, 2001, 291, 856-859.	12.6	358
146	Short- and intermediate-range structure of liquid GeSe2. Physical Review B, 2001, 64, .	3.2	77
147	Reconstruction of frozen-core all-electron orbitals from pseudo-orbitals. Journal of Chemical Physics, 2001, 115, 5791-5795.	3.0	32
148	Dangling Bond Defects atSiâˆ’SiO2Interfaces: Atomic Structure of thePb1Center. Physical Review Letters, 2000, 85, 2773-2776.	7.8	104
149	Concentration fluctuations on intermediate range distances in liquid GeSe2: the critical role of ionicity. Computational Materials Science, 2000, 17, 115-121.	3.0	15
150	First-principles molecular-dynamics study of the (0001)Î±âˆ’quartzsurface. Physical Review B, 2000, 61, 13250-13255.	3.2	142
151	Two-Dimensional Self-Assembly of Supramolecular Clusters and Chains. Physical Review Letters, 1999, 83, 324-327.	7.8	396
152	A comparison of methods for the calculation of NMR chemical shifts. Journal of Chemical Physics, 1999, 111, 1815-1822.	3.0	147
153	Intermediate Range Order and Bonding Character in Disordered Network-Forming Systems. Journal of the American Chemical Society, 1999, 121, 2943-2944.	13.7	59
154	Interface structure between silicon and its oxide by first-principles molecular dynamics. Nature, 1998, 396, 58-60.	27.8	230
155	Dynamics of structural relaxation upon Rydberg excitation of an impurity in an Ar crystal. Chemical Physics, 1998, 233, 343-352.	1.9	33
156	Fully Unconstrained Approach to Noncollinear Magnetism: Application to Small Fe Clusters. Physical Review Letters, 1998, 80, 3622-3625.	7.8	331
157	Identification of Raman Defect Lines as Signatures of Ring Structures in Vitreous Silica. Physical Review Letters, 1998, 80, 5145-5147.	7.8	377
158	Structure and electronic properties of amorphous indium phosphide from first principles. Physical Review B, 1998, 57, 1594-1606.	3.2	18
159	Microscopic Structure of LiquidGeSe2: The Problem of Concentration Fluctuations over Intermediate Range Distances. Physical Review Letters, 1998, 80, 2342-2345.	7.8	74
160	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
161	Cu++ and Li+ interaction with polyethylene oxide byab initiomolecular dynamics. Journal of Chemical Physics, 1998, 108, 9933-9936.	3.0	17
162	Nitrogen Incorporation atSi(001)âˆ’SiO2Interfaces: Relation between N1sCore-Level Shifts and Microscopic Structure. Physical Review Letters, 1997, 79, 5174-5177.	7.8	142

#	Article	IF	Citations
163	Structure and Hyperfine Parameters ofE1â€²Centers inÎ±-Quartz and in VitreousSiO2. Physical Review Letters, 1997, 78, 887-890.	7.8	207
164	Origin of the High-Frequency Doublet in the Vibrational Spectrum of Vitreous SiO2. Science, 1997, 275, 1925-1927.	12.6	133
165	Dynamical Charge Tensors and Infrared Spectrum of AmorphousSiO2. Physical Review Letters, 1997, 79, 1766-1769.	7.8	141
166	How hard spheres stack up. Nature, 1997, 385, 115-116.	27.8	6
167	Generalized-gradient approximations to density-functional theory: A comparative study for atoms and solids. Physical Review B, 1996, 53, 1180-1185.	3.2	228
168	Theory of Si 2pcore-level shifts at the Si(001)-SiO2interface. Physical Review B, 1996, 53, 10942-10950.	3.2	211
169	Structurally relaxed models of the Si(001)â€“SiO2 interface. Applied Physics Letters, 1996, 68, 625-627.	3.3	110
170	A microscopic model for surface-induced diamond-to-graphite transitions. Nature, 1996, 379, 523-526.	27.8	115
171	SpherosiloxaneH8Si8O12clusters on Si(001): First-principles calculation of Si2pcore-level shifts. Physical Review B, 1996, 54, R2339-R2342.	3.2	38
172	First-principles free-energy calculations on condensed-matter systems: Lattice vacancy in silicon. Physical Review B, 1996, 53, 9760-9763.	3.2	16
173	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
174	Structural and electronic properties of small copper clusters: a first principles study. Chemical Physics Letters, 1995, 238, 215-221.	2.6	91
175	Ab InitioMolecular Dynamics Study of First-Order Phase Transitions: Melting of Silicon. Physical Review Letters, 1995, 74, 1823-1826.	7.8	246
176	First-Principles Study of Excitonic Self-Trapping in Diamond. Physical Review Letters, 1995, 75, 3166-3169.	7.8	67
177	Si2pCore-Level Shifts at the Si(001)-SiO2Interface: A First-Principles Study. Physical Review Letters, 1995, 74, 1024-1027.	7.8	179
178	Model of vitreousSiO2generated by anab initiomolecular-dynamics quench from the melt. Physical Review B, 1995, 52, 12690-12695.	3.2	180
179	First Principles Study of Photoelectron Spectra ofCunâ^'Clusters. Physical Review Letters, 1995, 75, 2104-2107.	7.8	66
180	Structural and Electronic Properties of Liquid and Amorphous SiO2: AnAb InitioMolecular Dynamics Study. Physical Review Letters, 1995, 74, 4682-4685.	7.8	266

#	Article	IF	Citations
181	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
182	Ab initiostudy of positron trapping at a vacancy in GaAs. Physical Review Letters, 1994, 72, 3214-3217.	7.8	67
183	Diffusion mechanism of Cu adatoms on a Cu(001) surface. Surface Science, 1994, 306, L575-L578.	1.9	54
184	Orbital formulation for electronic-structure calculations with linear system-size scaling. Physical Review B, 1993, 47, 9973-9976.	3.2	436
185	Car-Parrinello molecular dynamics with Vanderbilt ultrasoft pseudopotentials. Physical Review B, 1993, 47, 10142-10153.	3.2	1,303
186	Auxiliary-field quantum Monte Carlo calculations for systems with long-range repulsive interactions. Physical Review Letters, 1993, 71, 1148-1151.	7.8	32
187	Ab initiomolecular dynamics ford-electron systems: Liquid copper at 1500 K. Physical Review Letters, 1992, 69, 1982-1985.	7.8	346
188	Implementation of ultrasoft pseudopotentials inab initiomolecular dynamics. Physical Review B, 1991, 43, 6796-6799.	3.2	453
189	Structure, growth, and bonding nature of Mg clusters. Physical Review B, 1991, 44, 8243-8255.	3.2	96
190	Ab initiocalculation of properties of carbon in the amorphous and liquid states. Physical Review B, 1990, 42, 7470-7482.	3.2	258
191	First-Principles Molecular Dynamics Simulations of Disordered Materials. Europhysics News, 1989, 20, 69-72.	0.3	0
192	Carbon: The nature of the liquid state. Physical Review Letters, 1989, 63, 988-991.	7.8	113
193	Structural and Electronic Properties of Amorphous Carbon. Physical Review Letters, 1989, 62, 555-558.	7.8	301
194	Equilibrium Structures and Finite Temperature Properties of Silicon Microclusters fromab initioMolecular-Dynamics Calculations. Physical Review Letters, 1988, 60, 271-274.	7.8	279
195	Role of electron-hole interactions in the optical spectra of metals. Physical Review Letters, 1987, 58, 1367-1370.	7.8	2
196	Energy-gap reduction in heavily doped silicon: Causes and consequences. Solid-State Electronics, 1985, 28, 17-24.	1.4	60
197	Electronic and structural properties of sodium clusters. Physical Review B, 1985, 31, 1804-1816.	3.2	352
198	Microscopic Theory of Impurity-Defect Reactions and Impurity Diffusion in Silicon. Physical Review Letters, 1985, 54, 360-363.	7.8	146

#	Article	IF	Citations
199	Forces in pseudopotential molecular calculations. Journal of Chemical Physics, 1984, 80, 1525-1528.	3.0	8
200	Theory of electronically stimulated defect migration in semiconductors. Physical Review B, 1984, 30, 2260-2262.	3.2	33
201	Equilibrium Geometries and Electronic Structures of Small Sodium Clusters. Physical Review Letters, 1984, 53, 655-658.	7.8	76
202	Electronic properties of alkali trimers. Journal of Chemical Physics, 1983, 78, 5646-5655.	3.0	184