Roberto Car

List of Publications by Year in Descending Order

198 papers	41,068 citations	72 h-index	202 g-index
204 ext. papers	45,887 ext. citations	7.3 avg, IF	7.12 L-index

#	Paper	IF	Citations
198	A deep potential model with long-range electrostatic interactions.. *Journal of Chemical Physics*, **2022**, 156, 124107	3.9	7
197	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	11.5	3
196	Heat transport in liquid water from first-principles and deep neural network simulations. *Physical Review B*, **2021**, 104,	3.3	4
195	Phase Equilibrium of Water with Hexagonal and Cubic Ice Using the SCAN Functional. *Journal of Chemical Theory and Computation*, **2021**, 17, 3065-3077	6.4	14
194	Band Engineering of Dirac Semimetals Using Charge Density Waves. *Advanced Materials*, **2021**, 33, e2101591	27	6
193	Phase Diagram of a Deep Potential Water Model. *Physical Review Letters*, **2021**, 126, 236001	7.4	27
192	Manifestations of metastable criticality in the long-range structure of model water glasses. *Nature Communications*, **2021**, 12, 3398	17.4	7
191	86 PFLOPS Deep Potential Molecular Dynamics simulation of 100 million atoms with ab initio accuracy. *Computer Physics Communications*, **2021**, 259, 107624	4.2	41
190	When do short-range atomistic machine-learning models fall short?. *Journal of Chemical Physics*, **2021**, 154, 034111	3.9	26
189	Monte Carlo Renormalization Group for Classical Lattice Models with Quenched Disorder. *Physical Review Letters*, **2020**, 125, 190601	7.4	
188	Raman spectrum and polarizability of liquid water from deep neural networks. *Physical Chemistry Chemical Physics*, **2020**, 22, 10592-10602	3.6	43
187	Phase equilibrium of liquid water and hexagonal ice from enhanced sampling molecular dynamics simulations. *Journal of Chemical Physics*, **2020**, 152, 204116	3.9	12
186	Quantum momentum distribution and quantum entanglement in the deep tunneling regime. *Journal of Chemical Physics*, **2020**, 152, 024106	3.9	0
185	Free energy of proton transfer at the water-TiO interface from deep potential molecular dynamics. *Chemical Science*, **2020**, 11, 2335-2341	9.4	60
184	Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based Molecular Dynamics. 1. Theory, Algorithm, and Performance. *Journal of Chemical Theory and Computation*, **2020**, 16, 3757-3785	6.4	13
183	Influence of point defects on the electronic and topological properties of monolayer WTe2. *Physical Review B*, **2020**, 102,	3.3	5
182	Pushing the Limit of Molecular Dynamics with Ab Initio Accuracy to 100 Million Atoms with Machine Learning **2020**,		29

181	Signatures of a liquid-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	11.5	45
180	Deep neural network for the dielectric response of insulators. *Physical Review B*, **2020**, 102,	3.3	32
179	Continuous-time Monte Carlo renormalization group. *Physical Review B*, **2020**, 102,	3.3	1
178	Hydrogen Dynamics in Supercritical Water Probed by Neutron Scattering and Computer Simulations. *Journal of Physical Chemistry Letters*, **2020**, 11, 9461-9467	6.4	6
177	Quantum ESPRESSO toward the exascale. *Journal of Chemical Physics*, **2020**, 152, 154105	3.9	227
176	Determination of the critical manifold tangent space and curvature with Monte Carlo renormalization group. *Physical Review E*, **2019**, 100, 022138	2.4	2
175	Isotope effects in liquid water via deep potential molecular dynamics. *Molecular Physics*, **2019**, 117, 3269-3281	1.7	35
174	Active learning of uniformly accurate interatomic potentials for materials simulation. *Physical Review Materials*, **2019**, 3,	3.2	154
173	Reliable and practical computational description of molecular crystal polymorphs. *Science Advances* , **2019**, 5, eaau3338	14.3	83
172	Prediction of a magnetic Weyl semimetal without spin-orbit coupling and strong anomalous Hall effect in the Heusler compensated ferrimagnet Ti2MnAl. *Physical Review B*, **2018**, 97,	3.3	43
171	Deep Potential Molecular Dynamics: A Scalable Model with the Accuracy of Quantum Mechanics. *Physical Review Letters*, **2018**, 120, 143001	7.4	488
170	Comment on "The putative liquid-liquid transition is a liquid-solid transition in atomistic models of water" [I and II: J. Chem. Phys. 135, 134503 (2011); J. Chem. Phys. 138, 214504 (2013)]. *Journal of Chemical Physics*, **2018**, 148, 137101	3.9	50
169	Local-order metric for condensed-phase environments. *Physical Review B*, **2018**, 97,	3.3	31
168	Hydroxide diffuses slower than hydronium in water because its solvated structure inhibits correlated proton transfer. *Nature Chemistry*, **2018**, 10, 413-419	17.6	124
167	DeePCG: Constructing coarse-grained models via deep neural networks. *Journal of Chemical Physics* , **2018**, 149, 034101	3.9	85
166	Thermal expansion in dispersion-bound molecular crystals. *Physical Review Materials*, **2018**, 2,	3.2	14
165	Searching for crystal-ice domains in amorphous ices. *Physical Review Materials*, **2018**, 2,	3.2	29
164	Deep Potential: A General Representation of a Many-Body Potential Energy Surface. *Communications in Computational Physics*, **2018**, 23,	2.4	82

163	From Colossal to Zero: Controlling the Anomalous Hall Effect in Magnetic Heusler Compounds via Berry Curvature Design. *Physical Review X*, **2018**, 8,	9.1	37
162	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	1.2	0
161	Structure, Polarization, and Sum Frequency Generation Spectrum of Interfacial Water on Anatase TiO. *Journal of Physical Chemistry Letters*, **2018**, 9, 6716-6721	6.4	51
160	Root-growth of boron nitride nanotubes: experiments and ab initio simulations. *Nanoscale*, **2018**, 10, 22223-22230	7.7	14
159	In situ Characterization of Nanoparticles Using Rayleigh Scattering. *Scientific Reports*, **2017**, 7, 40230	4.9	17
158	Assessment of the Tao-Mo nonempirical semilocal density functional in applications to solids and surfaces. *Physical Review B*, **2017**, 95,	3.3	32
157	Migration of a carbon adatom on a charged single-walled carbon nanotube. *Carbon*, **2017**, 116, 174-180	10.4	9
156	Large-Scale Structure and Hyperuniformity of Amorphous Ices. *Physical Review Letters*, **2017**, 119, 136001	7.4	31
155	Ab initio theory and modeling of water. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 10846-10851	11.5	246
154	Variational Approach to Monte Carlo Renormalization Group. *Physical Review Letters*, **2017**, 119, 220602	7.4	9
153	Density functional theory: Fixing Jacob's ladder. *Nature Chemistry*, **2016**, 8, 820-1	17.6	30
152	Fermionic Symmetry-Protected Topological Phase in a Two-Dimensional Hubbard Model. *Physical Review Letters*, **2016**, 117, 096405	7.4	4
151	Report on the sixth blind test of organic crystal structure prediction methods. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 439-59	1.8	338
150	Inverse design of disordered stealthy hyperuniform spin chains. *Physical Review B*, **2016**, 93,	3.3	12
149	A well-scaling natural orbital theory. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 12913-12918	11.5	10
148	Palmer et al. reply. *Nature*, **2016**, 531, E2-3	50.4	14
147	Analytical nuclear gradients for the range-separated many-body dispersion model of noncovalent interactions. *Chemical Science*, **2016**, 7, 1712-1728	9.4	29
146	Topological Nonsymmorphic Metals from Band Inversion. *Physical Review X*, **2016**, 6,	9.1	48

145	Performance of a nonempirical density functional on molecules and hydrogen-bonded complexes. *Journal of Chemical Physics*, **2016**, 145, 234306	3.9	23
144	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	3.8	97
143	Electronic properties of molecules and surfaces with a self-consistent interatomic van der Waals density functional. *Physical Review Letters*, **2015**, 114, 176802	7.4	72
142	The phase diagram of high-pressure superionic ice. *Nature Communications*, **2015**, 6, 8156	17.4	39
141	Local structure analysis in ab initio liquid water. *Molecular Physics*, **2015**, 113, 2829-2841	1.7	83
140	Metastable liquid-liquid transition in a molecular model of water. *Nature*, **2014**, 510, 385-8	50.4	356
139	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	3.9	223
138	MBius molecules and fragile Mott insulators. *Physical Review B*, **2014**, 90,	3.3	1
137	The liquid-liquid transition in supercooled ST2 water: a comparison between umbrella sampling and well-tempered metadynamics. *Faraday Discussions*, **2013**, 167, 77-94	3.6	71
136	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, 2017-22	11.5	6
135	Designer spin systems via inverse statistical mechanics. *Physical Review B*, **2013**, 88,	3.3	13
134	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	3.9	107
133	Enhanced thermal decomposition of nitromethane on functionalized graphene sheets: ab initio molecular dynamics simulations. *Journal of the American Chemical Society*, **2012**, 134, 19011-6	16.4	72
132	PHONON-INDUCED ANISOTROPIC DISPERSION FORCES ON A METALLIC SUBSTRATE. *Nano LIFE*, **2012**, 02, 1240001	0.9	2
131	Roles of quantum nuclei and inhomogeneous screening in the x-ray absorption spectra of water and ice. *Physical Review B*, **2012**, 86,	3.3	48
130	Accurate and efficient method for many-body van der Waals interactions. *Physical Review Letters*, **2012**, 108, 236402	7.4	920
129	Simple, unambiguous theoretical approach to oxidation state determination via first-principles calculations. *Inorganic Chemistry*, **2011**, 50, 10259-67	5.1	83
128	Correlated Tunneling in Hydrogen Bonds. *Journal of Statistical Physics*, **2011**, 145, 365-384	1.5	37

127	Oxidation state changes and electron flow in enzymatic catalysis and electrocatalysis through Wannier-function analysis. *Chemistry - A European Journal*, **2011**, 17, 12136-43	4.8	28
126	Electrocatalyst design from first principles: A hydrogen-production catalyst inspired by nature. *Catalysis Today*, **2011**, 165, 160-170	5.3	5
125	Hydrogen bonds and van der waals forces in ice at ambient and high pressures. *Physical Review Letters*, **2011**, 107, 185701	7.4	181
124	Effect of disorder on spin-transfer torque in magnetic tunnel junctions. *Journal of Applied Physics*, **2011**, 109, 07C920	2.5	3
123	Momentum distribution, vibrational dynamics, and the potential of mean force in ice. *Physical Review B*, **2011**, 83,	3.3	32
122	Displaced path integral formulation for the momentum distribution of quantum particles. *Physical Review Letters*, **2010**, 105, 110602	7.4	47
121	Theoretical Design by First Principles Molecular Dynamics of a Bioinspired Electrode-Catalyst System for Electrocatalytic Hydrogen Production from Acidified Water. *Journal of Chemical Theory and Computation*, **2010**, 6, 3490-502	6.4	13
120	X-ray absorption signatures of the molecular environment in water and ice. *Physical Review Letters*, **2010**, 105, 017802	7.4	79
119	Influence of asymmetry on bias behavior of spin torque. *Physical Review B*, **2010**, 81,	3.3	43
118	Simulation of electrocatalytic hydrogen production by a bioinspired catalyst anchored to a pyrite electrode. *Journal of the American Chemical Society*, **2010**, 132, 8593-601	16.4	30
117	Order-N implementation of exact exchange in extended insulating systems. *Physical Review B*, **2009** , 79,	3.3	151
116	Theory of tunneling transport in periodic chains. *Physical Review B*, **2009**, 80,	3.3	11
115	Tunneling and delocalization effects in hydrogen bonded systems: a study in position and momentum space. *Journal of Chemical Physics*, **2009**, 130, 204511	3.9	62
114	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. *Journal of Physics Condensed Matter*, **2009**, 21, 395502	1.8	13251
113	Hydrogen production by the naked active site of the di-iron hydrogenases in water. *Journal of Physical Chemistry B*, **2009**, 113, 13096-106	3.4	10
112	Hybrid density functional calculations of the band gap of GaxIn1⊠N. *Physical Review B*, **2009**, 80,	3.3	39
111	Charge transfer in partition theory. *Journal of Physical Chemistry A*, **2009**, 113, 2183-92	2.8	10
110	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	41

109	Bending properties of single functionalized graphene sheets probed by atomic force microscopy. *ACS Nano*, **2008**, 2, 2577-84	16.7	167
108	Mechanism of H2 production by the [FeFe]H subcluster of di-iron hydrogenases: implications for abiotic catalysts. *Journal of Physical Chemistry B*, **2008**, 112, 13381-90	3.4	10
107	Structures, Interactions, and Ferromagnetism of Fe□arbon Nanotube Systems. *Journal of Physical Chemistry C*, **2008**, 112, 8400-8407	3.8	12
106	Dynamical optimization for partition theory. *Journal of Physical Chemistry A*, **2008**, 112, 571-5	2.8	2
105	Tunneling conductance of amine-linked alkyl chains. *Nano Letters*, **2008**, 8, 1771-7	11.5	22
104	Role of dipolar correlations in the infrared spectra of water and ice. *Physical Review B*, **2008**, 77,	3.3	59
103	Band alignment in molecular devices: Influence of anchoring group and metal work function. *Physical Review B*, **2008**, 77,	3.3	32
102	Nuclear quantum effects in water. *Physical Review Letters*, **2008**, 101, 017801	7.4	324
101	Raman spectra of graphite oxide and functionalized graphene sheets. *Nano Letters*, **2008**, 8, 36-41	11.5	3540
100	Why are water-hydrophobic interfaces charged?. *Journal of the American Chemical Society*, **2008**, 130, 3915-9	16.4	167
99	Theoretical studies of [FeFe]-hydrogenase: infrared fingerprints of the dithiol-bridging ligand in the active site. *Inorganic Chemistry*, **2007**, 46, 1153-61	5.1	12
98	Dipolar correlations and the dielectric permittivity of water. *Physical Review Letters*, **2007**, 98, 247401	7.4	138
97	Single Sheet Functionalized Graphene by Oxidation and Thermal Expansion of Graphite. *Chemistry of Materials*, **2007**, 19, 4396-4404	9.6	2986
96	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	3.9	22
95	Quantization of the dipole moment and of the end charges in push-pull polymers. *Journal of Chemical Physics*, **2007**, 127, 194902	3.9	30
94	Proton momentum distribution in water: an open path integral molecular dynamics study. *Journal of Chemical Physics*, **2007**, 126, 234504	3.9	64
93	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, 2626-30	11.5	67
92	Electronic structure and reactivity of isomeric oxo-Mn(V) porphyrins: effects of spin-state crossing and pKa modulation. *Inorganic Chemistry*, **2006**, 45, 4268-76	5.1	101

91	Tuning the photoinduced O2-evolving reactivity of Mn4O47+, Mn4O46+, and Mn4O3(OH)6+ manganese-oxo cubane complexes. *Inorganic Chemistry*, **2006**, 45, 189-95	5.1	54
90	Anisotropic adsorption of molecular assemblies on crystalline surfaces. *Journal of Physical Chemistry B*, **2006**, 110, 16624-32	3.4	31
89	Oxygen-driven unzipping of graphitic materials. *Physical Review Letters*, **2006**, 96, 176101	7.4	477
88	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	3.9	39
87	Resolving the CO/CN ligand arrangement in CO-inactivated [FeFe] hydrogenase by first principles density functional theory calculations. *Inorganic Chemistry*, **2006**, 45, 5715-7	5.1	26
86	Orbital energetics and molecular recognition. *Journal of the American Chemical Society*, **2006**, 128, 4514-5	6.4	1
85	Theoretical studies of [FeFe]-hydrogenase: structure and infrared spectra of synthetic models. *Journal of Physical Chemistry B*, **2006**, 110, 7049-57	3.4	23
84	Functionalized single graphene sheets derived from splitting graphite oxide. *Journal of Physical Chemistry B*, **2006**, 110, 8535-9	3.4	2925
83	Intermolecular dynamical charge fluctuations in water: a signature of the H-bond network. *Physical Review Letters*, **2005**, 95, 187401	7.4	121
82	Quantum chemical evaluation of protein control over heme ligation: CO/O2 discrimination in myoglobin. *Journal of Physical Chemistry B*, **2005**, 109, 3065-70	3.4	49
81	A theoretical study of biotin chemisorption on Si-SiC(001) surfaces. *Journal of Physical Chemistry B*, **2005**, 109, 13656-62	3.4	19
80	Role of molecular conjugation in the surface radical reaction of aldehydes with H-Si(111): first principles study. *Journal of Physical Chemistry B*, **2005**, 109, 18889-94	3.4	30
79	Self-interstitial transport in vanadium. *Acta Materialia*, **2005**, 53, 1985-1994	8.4	18
78	Minimization of the potential energy surface of Lennard□Jones clusters by quantum optimization. *Chemical Physics Letters*, **2005**, 412, 125-130	2.5	12
77	Carbon phase diagram from ab initio molecular dynamics. *Physical Review Letters*, **2005**, 95, 185701	7.4	158
76	Electron transport with dissipation: A quantum kinetic approach. *International Journal of Quantum Chemistry*, **2005**, 101, 564-571	2.1	6
75	Longitudinal polarizability of long polymeric chains: quasi-one-dimensional electrostatics as the origin of slow convergence. *Journal of Chemical Physics*, **2005**, 122, 134907	3.9	21
74	Density functional theory of the electrical conductivity of molecular devices. *Physical Review Letters* , **2005**, 94, 146803	7.4	114

73	Free energy profile along a discretized reaction path via the hyperplane constraint force and torque. *Journal of Chemical Physics*, **2005**, 122, 114108	3.9	10
72	Use of dielectric functions in the theory of dispersion forces. *Physical Review B*, **2005**, 71,	3.3	43
71	Mapping potential energy surfaces. *Journal of Chemical Physics*, **2004**, 121, 1193-200	3.9	19
70	Current in open quantum systems. *Physical Review Letters*, **2004**, 93, 160404	7.4	56
69	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, 8632-7	3.9	137
68	The role of vacancy defects and holes in the fracture of carbon nanotubes. *Chemical Physics Letters*, **2004**, 390, 413-420	2.5	300
67	On the Mechanisms of OH Radical Induced DNA-Base Damage: A Comparative Quantum Chemical and Car□Parrinello Molecular Dynamics Study□ *Journal of Physical Chemistry A*, **2004**, 108, 2922-2929	2.8	51
66	Role of ligand bending in the photodissociation of O2 vs CO-heme: a time-dependent density functional study. *Journal of the American Chemical Society*, **2003**, 125, 15710-1	16.4	38
65	Ab initio molecular dynamics with maximally localized Wannier functions. *International Journal of Quantum Chemistry*, **2003**, 95, 821-829	2.1	49
64	Chemistry between magnesium and multiple molecules in tris(8-hydroxyquinoline) aluminum films. *Journal of the American Chemical Society*, **2003**, 125, 7808-9	16.4	31
63	Interatomic potential for vanadium suitable for radiation damage simulations. *Journal of Applied Physics*, **2003**, 93, 3328-3335	2.5	61
62	Closing of the nucleotide pocket of kinesin-family motors upon binding to microtubules. *Science*, **2003**, 300, 798-801	33.3	50
61	First-principles electronic structure study of Ti-PTCDA contacts. *Physical Review B*, **2002**, 65,	3.3	25
60	Pressure-induced structural changes in liquid SiO2 from Ab initio simulations. *Physical Review Letters*, **2002**, 89, 245504	7.4	83
59	Theory of quantum annealing of an Ising spin glass. *Science*, **2002**, 295, 2427-30	33.3	403
58	A classical and ab initio study of the interaction of the myosin triphosphate binding domain with ATP. *Biophysical Journal*, **2002**, 82, 660-75	2.9	33
57	Short- and intermediate-range structure of liquid GeSe2. *Physical Review B*, **2001**, 64,	3.3	75
56	Reconstruction of frozen-core all-electron orbitals from pseudo-orbitals. *Journal of Chemical Physics*, **2001**, 115, 5791-5795	3.9	30

55	First solvation shell of the Cu(II) aqua ion: evidence for fivefold coordination. *Science*, **2001**, 291, 856-9	33.3	314
54	Dangling bond defects at Si-SiO2 interfaces: atomic structure of the P(b1) center. *Physical Review Letters*, **2000**, 85, 2773-6	7.4	93
53	Concentration fluctuations on intermediate range distances in liquid GeSe2: the critical role of ionicity. *Computational Materials Science*, **2000**, 17, 115-121	3.2	14
52	First-principles molecular-dynamics study of the (0001) □quartz surface. *Physical Review B*, **2000**, 61, 13250-13255	3.3	126
51	Two-Dimensional Self-Assembly of Supramolecular Clusters and Chains. *Physical Review Letters*, **1999**, 83, 324-327	7.4	377
50	A comparison of methods for the calculation of NMR chemical shifts. *Journal of Chemical Physics*, **1999**, 111, 1815-1822	3.9	117
49	Intermediate Range Order and Bonding Character in Disordered Network-Forming Systems. *Journal of the American Chemical Society*, **1999**, 121, 2943-2944	16.4	57
48	Interface structure between silicon and its oxide by first-principles molecular dynamics. *Nature*, **1998**, 396, 58-60	50.4	209
47	Dynamics of structural relaxation upon Rydberg excitation of an impurity in an Ar crystal. *Chemical Physics*, **1998**, 233, 343-352	2.3	32
46	Fully Unconstrained Approach to Noncollinear Magnetism: Application to Small Fe Clusters. *Physical Review Letters*, **1998**, 80, 3622-3625	7.4	291
45	Identification of Raman Defect Lines as Signatures of Ring Structures in Vitreous Silica. *Physical Review Letters*, **1998**, 80, 5145-5147	7.4	337
44	Structure and electronic properties of amorphous indium phosphide from first principles. *Physical Review B*, **1998**, 57, 1594-1606	3.3	17
43	Microscopic Structure of Liquid GeSe2: The Problem of Concentration Fluctuations over Intermediate Range Distances. *Physical Review Letters*, **1998**, 80, 2342-2345	7.4	72
42	Dynamic structure factor of vitreous silica from first principles: Comparison to neutron-inelastic-scattering experiments. *Physical Review B*, **1998**, 57, 14133-14140	3.3	88
41	Cu++ and Li+ interaction with polyethylene oxide by ab initio molecular dynamics. *Journal of Chemical Physics*, **1998**, 108, 9933-9936	3.9	15
40	Nitrogen Incorporation at Si(001)□SiO2 Interfaces: Relation between N 1s Core-Level Shifts and Microscopic Structure. *Physical Review Letters*, **1997**, 79, 5174-5177	7.4	122
39	Structure and Hyperfine Parameters of E1? Centers in □Quartz and in Vitreous SiO2. *Physical Review Letters*, **1997**, 78, 887-890	7.4	194
38	Origin of the High-Frequency Doublet in the Vibrational Spectrum of Vitreous SiO2. *Science*, **1997**, 275, 1925-7	33.3	121

37	Dynamical Charge Tensors and Infrared Spectrum of Amorphous SiO2. *Physical Review Letters*, **1997**, 79, 1766-1769	7.4	133
36	Generalized-gradient approximations to density-functional theory: A comparative study for atoms and solids. *Physical Review B*, **1996**, 53, 1180-1185	3.3	204
35	Theory of Si 2p core-level shifts at the Si(001)-SiO2 interface. *Physical Review B*, **1996**, 53, 10942-10950	3.3	200
34	Structurally relaxed models of the Si(001)-SiO2 interface. *Applied Physics Letters*, **1996**, 68, 625-627	3.4	104
33	A microscopic model for surface-induced diamond-to-graphite transitions. *Nature*, **1996**, 379, 523-526	50.4	109
32	Spherosiloxane H8Si8O12 clusters on Si(001): First-principles calculation of Si 2p core-level shifts. *Physical Review B*, **1996**, 54, R2339-R2342	3.3	38
31	First-principles free-energy calculations on condensed-matter systems: Lattice vacancy in silicon. *Physical Review B*, **1996**, 53, 9760-9763	3.3	14
30	Interpretation of photoelectron spectra in Cun - clusters including thermal and final-state effects: The case of Cu7 -. *Physical Review B*, **1996**, 54, 8913-8918	3.3	25
29	Ab initio molecular dynamics study of first-order phase transitions: melting of silicon. *Physical Review Letters*, **1995**, 74, 1823-1826	7.4	207
28	First-principles study of excitonic self-trapping in diamond. *Physical Review Letters*, **1995**, 75, 3166-3169	7.4	61
27	Si 2p core-level shifts at the Si(001)-SiO2 interface: A first-principles study. *Physical Review Letters*, **1995**, 74, 1024-1027	7.4	174
26	Model of vitreous SiO2 generated by an ab initio molecular-dynamics quench from the melt. *Physical Review B*, **1995**, 52, 12690-12695	3.3	163
25	First principles study of photoelectron spectra of Cun- clusters. *Physical Review Letters*, **1995**, 75, 2104-2107	7.4	61
24	Structural and electronic properties of liquid and amorphous SiO2: An ab initio molecular dynamics study. *Physical Review Letters*, **1995**, 74, 4682-4685	7.4	251
23	Structural and electronic properties of small copper clusters: a first principles study. *Chemical Physics Letters*, **1995**, 238, 215-221	2.5	87
22	Low- and high-temperature phases of a Pb monolayer on Ge(111) from ab initio molecular dynamics. *Physical Review B*, **1994**, 50, 15158-15165	3.3	7
21	Ab initio study of positron trapping at a vacancy in GaAs. *Physical Review Letters*, **1994**, 72, 3214-3217	7.4	64
20	Diffusion mechanism of Cu adatoms on a Cu(001) surface. *Surface Science*, **1994**, 306, L575-L578	1.8	54

19	Car-Parrinello molecular dynamics with Vanderbilt ultrasoft pseudopotentials. *Physical Review B*, **1993**, 47, 10142-10153	3.3	1181
18	Auxiliary-field quantum Monte Carlo calculations for systems with long-range repulsive interactions. *Physical Review Letters*, **1993**, 71, 1148-1151	7.4	28
17	Orbital formulation for electronic-structure calculations with linear system-size scaling. *Physical Review B*, **1993**, 47, 9973-9976	3.3	388
16	Ab initio molecular dynamics for d-electron systems: Liquid copper at 1500 K. *Physical Review Letters*, **1992**, 69, 1982-1985	7.4	333
15	Implementation of ultrasoft pseudopotentials in ab initio molecular dynamics. *Physical Review B*, **1991**, 43, 6796-6799	3.3	382
14	Structure, growth, and bonding nature of Mg clusters. *Physical Review B*, **1991**, 44, 8243-8255	3.3	87
13	Ab initio calculation of properties of carbon in the amorphous and liquid states. *Physical Review B*, **1990**, 42, 7470-7482	3.3	225
12	Carbon: The nature of the liquid state. *Physical Review Letters*, **1989**, 63, 988-991	7.4	101
11	Structural and electronic properties of amorphous carbon. *Physical Review Letters*, **1989**, 62, 555-558	7.4	275
10	Equilibrium structures and finite temperature properties of silicon microclusters from ab initio molecular-dynamics calculations. *Physical Review Letters*, **1988**, 60, 271-274	7.4	258
9	Role of electron-hole interactions in the optical spectra of metals. *Physical Review Letters*, **1987**, 58, 1367-1370	7.4	2
8	Energy-gap reduction in heavily doped silicon: Causes and consequences. *Solid-State Electronics*, **1985**, 28, 17-24	1.7	54
7	Electronic and structural properties of sodium clusters. *Physical Review B*, **1985**, 31, 1804-1816	3.3	347
6	Microscopic theory of impurity-defect reactions and impurity diffusion in silicon. *Physical Review Letters*, **1985**, 54, 360-363	7.4	134
5	Forces in pseudopotential molecular calculations. *Journal of Chemical Physics*, **1984**, 80, 1525-1528	3.9	8
4	Theory of electronically stimulated defect migration in semiconductors. *Physical Review B*, **1984**, 30, 2260-2262	3.3	31
3	Equilibrium Geometries and Electronic Structures of Small Sodium Clusters. *Physical Review Letters*, **1984**, 53, 655-658	7.4	75
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