Roberto Car

List of Publications by Citations

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	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
197	Raman spectra of graphite oxide and functionalized graphene sheets. *Nano Letters*, **2008**, 8, 36-41	11.5	3540
196	Single Sheet Functionalized Graphene by Oxidation and Thermal Expansion of Graphite. *Chemistry of Materials*, **2007**, 19, 4396-4404	9.6	2986
195	Functionalized single graphene sheets derived from splitting graphite oxide. *Journal of Physical Chemistry B*, **2006**, 110, 8535-9	3.4	2925
194	Car-Parrinello molecular dynamics with Vanderbilt ultrasoft pseudopotentials. *Physical Review B*, **1993**, 47, 10142-10153	3.3	1181
193	Accurate and efficient method for many-body van der Waals interactions. *Physical Review Letters*, **2012**, 108, 236402	7.4	920
192	Deep Potential Molecular Dynamics: A Scalable Model with the Accuracy of Quantum Mechanics. *Physical Review Letters*, **2018**, 120, 143001	7.4	488
191	Oxygen-driven unzipping of graphitic materials. *Physical Review Letters*, **2006**, 96, 176101	7.4	477
190	Theory of quantum annealing of an Ising spin glass. *Science*, **2002**, 295, 2427-30	33.3	403
189	Orbital formulation for electronic-structure calculations with linear system-size scaling. *Physical Review B*, **1993**, 47, 9973-9976	3.3	388
188	Implementation of ultrasoft pseudopotentials in ab initio molecular dynamics. *Physical Review B*, **1991**, 43, 6796-6799	3.3	382
187	Two-Dimensional Self-Assembly of Supramolecular Clusters and Chains. *Physical Review Letters*, **1999**, 83, 324-327	7.4	377
186	Metastable liquid-liquid transition in a molecular model of water. *Nature*, **2014**, 510, 385-8	50.4	356
185	Electronic and structural properties of sodium clusters. *Physical Review B*, **1985**, 31, 1804-1816	3.3	347
184	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
183	Identification of Raman Defect Lines as Signatures of Ring Structures in Vitreous Silica. *Physical Review Letters*, **1998**, 80, 5145-5147	7.4	337
182	Ab initio molecular dynamics for d-electron systems: Liquid copper at 1500 K. *Physical Review Letters*, **1992**, 69, 1982-1985	7.4	333

181	Nuclear quantum effects in water. *Physical Review Letters*, **2008**, 101, 017801	7.4	324
180	First solvation shell of the Cu(II) aqua ion: evidence for fivefold coordination. *Science*, **2001**, 291, 856-9	33.3	314
179	The role of vacancy defects and holes in the fracture of carbon nanotubes. *Chemical Physics Letters*, **2004**, 390, 413-420	2.5	300
178	Fully Unconstrained Approach to Noncollinear Magnetism: Application to Small Fe Clusters. *Physical Review Letters*, **1998**, 80, 3622-3625	7.4	291
177	Structural and electronic properties of amorphous carbon. *Physical Review Letters*, **1989**, 62, 555-558	7.4	275
176	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
175	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
174	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
173	Quantum ESPRESSO toward the exascale. *Journal of Chemical Physics*, **2020**, 152, 154105	3.9	227
172	Ab initio calculation of properties of carbon in the amorphous and liquid states. *Physical Review B*, **1990**, 42, 7470-7482	3.3	225
171	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
170	Interface structure between silicon and its oxide by first-principles molecular dynamics. *Nature*, **1998**, 396, 58-60	50.4	209
169	Ab initio molecular dynamics study of first-order phase transitions: melting of silicon. *Physical Review Letters*, **1995**, 74, 1823-1826	7.4	207
168	Generalized-gradient approximations to density-functional theory: A comparative study for atoms and solids. *Physical Review B*, **1996**, 53, 1180-1185	3.3	204
167	Theory of Si 2p core-level shifts at the Si(001)-SiO2 interface. *Physical Review B*, **1996**, 53, 10942-10950	3.3	200
166	Structure and Hyperfine Parameters of E1? Centers in □Quartz and in Vitreous SiO2. *Physical Review Letters*, **1997**, 78, 887-890	7.4	194
165	Hydrogen bonds and van der waals forces in ice at ambient and high pressures. *Physical Review Letters*, **2011**, 107, 185701	7.4	181
164	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

163	Electronic properties of alkali trimers. *Journal of Chemical Physics*, **1983**, 78, 5646-5655	3.9	172
162	Bending properties of single functionalized graphene sheets probed by atomic force microscopy. *ACS Nano*, **2008**, 2, 2577-84	16.7	167
161	Why are water-hydrophobic interfaces charged?. *Journal of the American Chemical Society*, **2008**, 130, 3915-9	16.4	167
160	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
159	Carbon phase diagram from ab initio molecular dynamics. *Physical Review Letters*, **2005**, 95, 185701	7.4	158
158	Active learning of uniformly accurate interatomic potentials for materials simulation. *Physical Review Materials*, **2019**, 3,	3.2	154
157	Order-N implementation of exact exchange in extended insulating systems. *Physical Review B*, **2009**, 79,	3.3	151
156	Dipolar correlations and the dielectric permittivity of water. *Physical Review Letters*, **2007**, 98, 247401	7.4	138
155	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
154	Microscopic theory of impurity-defect reactions and impurity diffusion in silicon. *Physical Review Letters*, **1985**, 54, 360-363	7.4	134
153	Dynamical Charge Tensors and Infrared Spectrum of Amorphous SiO2. *Physical Review Letters*, **1997**, 79, 1766-1769	7.4	133
152	First-principles molecular-dynamics study of the (0001) α-quartz surface. *Physical Review B*, **2000**, 61, 13250-13255	3.3	126
151	Hydroxide diffuses slower than hydronium in water because its solvated structure inhibits correlated proton transfer. *Nature Chemistry*, **2018**, 10, 413-419	17.6	124
150	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
149	Origin of the High-Frequency Doublet in the Vibrational Spectrum of Vitreous SiO2. *Science*, **1997**, 275, 1925-7	33.3	121
148	Intermolecular dynamical charge fluctuations in water: a signature of the H-bond network. *Physical Review Letters*, **2005**, 95, 187401	7.4	121
147	A comparison of methods for the calculation of NMR chemical shifts. *Journal of Chemical Physics*, **1999**, 111, 1815-1822	3.9	117
146	Density functional theory of the electrical conductivity of molecular devices. *Physical Review Letters*, **2005**, 94, 146803	7.4	114

145	A microscopic model for surface-induced diamond-to-graphite transitions. *Nature*, **1996**, 379, 523-526	50.4	109
144	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
143	Structurally relaxed models of the Si(001)SiO2 interface. *Applied Physics Letters*, **1996**, 68, 625-627	3.4	104
142	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
141	Carbon: The nature of the liquid state. *Physical Review Letters*, **1989**, 63, 988-991	7.4	101
140	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
139	Dangling bond defects at Si-SiO2 interfaces: atomic structure of the P(b1) center. *Physical Review Letters*, **2000**, 85, 2773-6	7.4	93
138	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
137	Structural and electronic properties of small copper clusters: a first principles study. *Chemical Physics Letters*, **1995**, 238, 215-221	2.5	87
136	Structure, growth, and bonding nature of Mg clusters. *Physical Review B*, **1991**, 44, 8243-8255	3.3	87
135	DeePCG: Constructing coarse-grained models via deep neural networks. *Journal of Chemical Physics* , **2018**, 149, 034101	3.9	85
134	Local structure analysis in ab initio liquid water. *Molecular Physics*, **2015**, 113, 2829-2841	1.7	83
133	Simple, unambiguous theoretical approach to oxidation state determination via first-principles calculations. *Inorganic Chemistry*, **2011**, 50, 10259-67	5.1	83
132	Pressure-induced structural changes in liquid SiO2 from Ab initio simulations. *Physical Review Letters*, **2002**, 89, 245504	7.4	83
131	Reliable and practical computational description of molecular crystal polymorphs. *Science Advances* , **2019**, 5, eaau3338	14.3	83
130	Deep Potential: A General Representation of a Many-Body Potential Energy Surface. *Communications in Computational Physics*, **2018**, 23,	2.4	82
129	X-ray absorption signatures of the molecular environment in water and ice. *Physical Review Letters*, **2010**, 105, 017802	7.4	79
128	Short- and intermediate-range structure of liquid GeSe2. *Physical Review B*, **2001**, 64,	3.3	75

127	Equilibrium Geometries and Electronic Structures of Small Sodium Clusters. *Physical Review Letters*, **1984**, 53, 655-658	7.4	75
126	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
125	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
124	Microscopic Structure of Liquid GeSe2: The Problem of Concentration Fluctuations over Intermediate Range Distances. *Physical Review Letters*, **1998**, 80, 2342-2345	7.4	72
123	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
122	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
121	Proton momentum distribution in water: an open path integral molecular dynamics study. *Journal of Chemical Physics*, **2007**, 126, 234504	3.9	64
120	Ab initio study of positron trapping at a vacancy in GaAs. *Physical Review Letters*, **1994**, 72, 3214-3217	7.4	64
119	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
118	Interatomic potential for vanadium suitable for radiation damage simulations. *Journal of Applied Physics*, **2003**, 93, 3328-3335	2.5	61
117	First-principles study of excitonic self-trapping in diamond. *Physical Review Letters*, **1995**, 75, 3166-3169	7.4	61
116	First principles study of photoelectron spectra of Cun- clusters. *Physical Review Letters*, **1995**, 75, 2104-2107	7.4	61
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114	Role of dipolar correlations in the infrared spectra of water and ice. *Physical Review B*, **2008**, 77,	3.3	59
113	Intermediate Range Order and Bonding Character in Disordered Network-Forming Systems. *Journal of the American Chemical Society*, **1999**, 121, 2943-2944	16.4	57
112	Current in open quantum systems. *Physical Review Letters*, **2004**, 93, 160404	7.4	56
111	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
110	Diffusion mechanism of Cu adatoms on a Cu(001) surface. *Surface Science*, **1994**, 306, L575-L578	1.8	54

109	Energy-gap reduction in heavily doped silicon: Causes and consequences. *Solid-State Electronics*, **1985**, 28, 17-24	1.7	54
108	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
107	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
106	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
105	Closing of the nucleotide pocket of kinesin-family motors upon binding to microtubules. *Science*, **2003**, 300, 798-801	33.3	50
104	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
103	Ab initio molecular dynamics with maximally localized Wannier functions. *International Journal of Quantum Chemistry*, **2003**, 95, 821-829	2.1	49
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101	Topological Nonsymmorphic Metals from Band Inversion. *Physical Review X*, **2016**, 6,	9.1	48
100	Displaced path integral formulation for the momentum distribution of quantum particles. *Physical Review Letters*, **2010**, 105, 110602	7.4	47
99	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
98	Raman spectrum and polarizability of liquid water from deep neural networks. *Physical Chemistry Chemical Physics*, **2020**, 22, 10592-10602	3.6	43
97	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
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95	Use of dielectric functions in the theory of dispersion forces. *Physical Review B*, **2005**, 71,	3.3	43
94	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
93	86 PFLOPS Deep Potential Molecular Dynamics simulation of 100 million atoms with ab initio accuracy. *Computer Physics Communications*, **2021**, 259, 107624	4.2	41
92	The phase diagram of high-pressure superionic ice. *Nature Communications*, **2015**, 6, 8156	17.4	39

91	Hybrid density functional calculations of the band gap of GaxIn1⊠N. *Physical Review B*, **2009**, 80,	3.3	39
90	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
89	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
88	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
87	Correlated Tunneling in Hydrogen Bonds. *Journal of Statistical Physics*, **2011**, 145, 365-384	1.5	37
86	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
85	Isotope effects in liquid water via deep potential molecular dynamics. *Molecular Physics*, **2019**, 117, 3269-3281	1.7	35
84	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
83	Assessment of the Tao-Mo nonempirical semilocal density functional in applications to solids and surfaces. *Physical Review B*, **2017**, 95,	3.3	32
82	Momentum distribution, vibrational dynamics, and the potential of mean force in ice. *Physical Review B*, **2011**, 83,	3.3	32
81	Dynamics of structural relaxation upon Rydberg excitation of an impurity in an Ar crystal. *Chemical Physics*, **1998**, 233, 343-352	2.3	32
80	Band alignment in molecular devices: Influence of anchoring group and metal work function. *Physical Review B*, **2008**, 77,	3.3	32
79	Deep neural network for the dielectric response of insulators. *Physical Review B*, **2020**, 102,	3.3	32
78	Large-Scale Structure and Hyperuniformity of Amorphous Ices. *Physical Review Letters*, **2017**, 119, 136002	7.4	31
77	Local-order metric for condensed-phase environments. *Physical Review B*, **2018**, 97,	3.3	31
76	Anisotropic adsorption of molecular assemblies on crystalline surfaces. *Journal of Physical Chemistry B*, **2006**, 110, 16624-32	3.4	31
75	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
74	Theory of electronically stimulated defect migration in semiconductors. *Physical Review B*, **1984**, 30, 2260-2262	3.3	31

73	Density functional theory: Fixing Jacob's ladder. *Nature Chemistry*, **2016**, 8, 820-1	17.6	30
72	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
71	Quantization of the dipole moment and of the end charges in push-pull polymers. *Journal of Chemical Physics*, **2007**, 127, 194902	3.9	30
70	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
69	Reconstruction of frozen-core all-electron orbitals from pseudo-orbitals. *Journal of Chemical Physics*, **2001**, 115, 5791-5795	3.9	30
68	Analytical nuclear gradients for the range-separated many-body dispersion model of noncovalent interactions. *Chemical Science*, **2016**, 7, 1712-1728	9.4	29
67	Searching for crystal-ice domains in amorphous ices. *Physical Review Materials*, **2018**, 2,	3.2	29
66	Pushing the Limit of Molecular Dynamics with Ab Initio Accuracy to 100 Million Atoms with Machine Learning **2020**,		29
65	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
64	Auxiliary-field quantum Monte Carlo calculations for systems with long-range repulsive interactions. *Physical Review Letters*, **1993**, 71, 1148-1151	7.4	28
63	Phase Diagram of a Deep Potential Water Model. *Physical Review Letters*, **2021**, 126, 236001	7.4	27
62	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
61	When do short-range atomistic machine-learning models fall short?. *Journal of Chemical Physics*, **2021**, 154, 034111	3.9	26
60	First-principles electronic structure study of Ti-PTCDA contacts. *Physical Review B*, **2002**, 65,	3.3	25
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58	Theoretical studies of [FeFe]-hydrogenase: structure and infrared spectra of synthetic models. *Journal of Physical Chemistry B*, **2006**, 110, 7049-57	3.4	23
57	Performance of a nonempirical density functional on molecules and hydrogen-bonded complexes. *Journal of Chemical Physics*, **2016**, 145, 234306	3.9	23
56	Tunneling conductance of amine-linked alkyl chains. *Nano Letters*, **2008**, 8, 1771-7	11.5	22

55	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
54	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
53	A theoretical study of biotin chemisorption on Si-SiC(001) surfaces. *Journal of Physical Chemistry B*, **2005**, 109, 13656-62	3.4	19
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51	Self-interstitial transport in vanadium. *Acta Materialia*, **2005**, 53, 1985-1994	8.4	18
50	In situ Characterization of Nanoparticles Using Rayleigh Scattering. *Scientific Reports*, **2017**, 7, 40230	4.9	17
49	Structure and electronic properties of amorphous indium phosphide from first principles. *Physical Review B*, **1998**, 57, 1594-1606	3.3	17
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41	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
40	Designer spin systems via inverse statistical mechanics. *Physical Review B*, **2013**, 88,	3.3	13
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34	Minimization of the potential energy surface of Lennard–Jones clusters by quantum optimization. *Chemical Physics Letters*, **2005**, 412, 125-130	2.5	12
33	Theory of tunneling transport in periodic chains. *Physical Review B*, **2009**, 80,	3.3	11
32	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
31	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
30	Charge transfer in partition theory. *Journal of Physical Chemistry A*, **2009**, 113, 2183-92	2.8	10
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24	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
23	Manifestations of metastable criticality in the long-range structure of model water glasses. *Nature Communications*, **2021**, 12, 3398	17.4	7
22	A deep potential model with long-range electrostatic interactions.. *Journal of Chemical Physics*, **2022**, 156, 124107	3.9	7
21	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
20	Electron transport with dissipation: A quantum kinetic approach. *International Journal of Quantum Chemistry*, **2005**, 101, 564-571	2.1	6

19	Hydrogen Dynamics in Supercritical Water Probed by Neutron Scattering and Computer Simulations. *Journal of Physical Chemistry Letters*, **2020**, 11, 9461-9467	6.4	6
18	Band Engineering of Dirac Semimetals Using Charge Density Waves. *Advanced Materials*, **2021**, 33, e2101591	25	6
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14	Heat transport in liquid water from first-principles and deep neural network simulations. *Physical Review B*, **2021**, 104,	3.3	4
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