Dario AlfÃ¨

List of Publications by Year
in descending order

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214 papers	13,719 citations	17440 63 h-index	24982 109 g-index
218 all docs	218 docs citations	218 times ranked	10472 citing authors

#	Article	IF	Citations
1	PHON: A program to calculate phonons using the small displacement method. Computer Physics Communications, 2009, 180, 2622-2633.	7.5	664
2	Perspective: How good is DFT for water?. Journal of Chemical Physics, 2016, 144, 130901.	3.0	571
3	Thermal and electrical conductivity of iron at Earthâ€™s core conditions. Nature, 2012, 485, 355-358.	27.8	510
4	Stone-Wales defects in graphene and other planar<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>s</mml:mi><mml:msup><mml:mi>p</mml:mi><mml:mn>2</mml:mn></mml:msup></mml:mrow materials. Physical Review B, 2009, 80, .	3.2	422
5	Hydrogen dissociation and diffusion on transition metal (=Ti, Zr, V, Fe, Ru, Co, Rh, Ni, Pd, Cu, Ag)-doped Mg(0001) surfaces. International Journal of Hydrogen Energy, 2009, 34, 1922-1930.	7.1	331
6	Phonon Density of States of Iron up to 153 Gigapascals. Science, 2001, 292, 914-916.	12.6	284
7	Iron under Earthâ€™s core conditions: Liquid-state thermodynamics and high-pressure melting curve fromab initiocalculations. Physical Review B, 2002, 65, .	3.2	277
8	The melting curve of iron at the pressures of the Earth's core from ab initio calculations. Nature, 1999, 401, 462-464.	27.8	270
9	The viscosity of liquid iron at the physical conditions of the Earth's core. Nature, 1998, 392, 805-807.	27.8	259
10	Composition and temperature of the Earthâ€™s core constrained by combining ab initio calculations and seismic data. Earth and Planetary Science Letters, 2002, 195, 91-98.	4.4	257
11	Thermodynamics of hexagonal-close-packed iron under Earthâ€™s core conditions. Physical Review B, 2001, 64, .	3.2	252
12	Possible thermal and chemical stabilization of body-centred-cubic iron in the Earth's core. Nature, 2003, 424, 536-539.	27.8	249
13	Structure and dynamics of liquid iron under Earthâ€™s core conditions. Physical Review B, 2000, 61, 132-142.	3.2	245
14	Adsorption and diffusion of water on graphene from first principles. Physical Review B, 2011, 84, .	3.2	218
15	Hydrogen Bonds and van der Waals Forces in Ice at Ambient and High Pressures. Physical Review Letters, 2011, 107, 185701.	7.8	193
16	Growth of Dome-Shaped Carbon Nanoislands on Ir(111): The Intermediate between Carbidic Clusters and Quasi-Free-Standing Graphene. Physical Review Letters, 2009, 103, 166101.	7.8	178
17	First-Principles Calculation of Transport Coefficients. Physical Review Letters, 1998, 81, 5161-5164.	7.8	170
18	Hard Numbers for Large Molecules: Toward Exact Energetics for Supramolecular Systems. Journal of Physical Chemistry Letters, 2014, 5, 849-855.	4.6	159

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19	Melting Curve of MgO from First-Principles Simulations. Physical Review Letters, 2005, 94, 235701.	7.8	158
20	First-principles modelling of Earth and planetary materials at high pressures and temperatures. Reports on Progress in Physics, 2006, 69, 2365-2441.	20.1	152
21	Thermal Expansion of Supported and Freestanding Graphene: Lattice Constant versus Interatomic Distance. Physical Review Letters, 2011, 106, 135501.	7.8	148
22	Development of a machine learning potential for graphene. Physical Review B, 2018, 97, .	3.2	142
23	The properties of iron under core conditions from first principles calculations. Physics of the Earth and Planetary Interiors, 2003, 140, 101-125.	1.9	138
24	Temperature of the inner-core boundary of the Earth: Melting of iron at high pressure from first-principles coexistence simulations. Physical Review B, 2009, 79, .	3.2	136
25	Gross thermodynamics of two-component core convection. Geophysical Journal International, 2004, 157, 1407-1414.	2.4	131
26	Transport properties for liquid silicon-oxygen-iron mixtures at Earth's core conditions. Physical Review B, 2013, 87, .	3.2	131
27	Can the Earth's dynamo run on heat alone?. Geophysical Journal International, 2003, 155, 609-622.	2.4	128
28	Ab initiomelting curve of the fcc phase of aluminum. Physical Review B, 2002, 65, .	3.2	124
29	Efficient localized basis set for quantum Monte Carlo calculations on condensed matter. Physical Review B, 2004, 70, .	3.2	122
30	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
31	Crucial role of atomic corrugation on the flat bands and energy gaps of twisted bilayer graphene at the magic angle <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î¸</mml:mi><mml:mo>â‰¼</mml:mo><mml:mn>1</mml:mn> Physical Review B, 2019, 99, .	3.2	119
32	Constraints from material properties on the dynamics and evolution of Earthâ€™s core. Nature Geoscience, 2015, 8, 678-685.	12.9	117
33	Thermal and electrical conductivity of solid iron and ironâ€“silicon mixtures at Earth's core conditions. Earth and Planetary Science Letters, 2014, 393, 159-164.	4.4	110
34	Comparative study of water dissociation on Rh(111) and Ni(111) studied with first principles calculations. Journal of Chemical Physics, 2007, 126, 164706.	3.0	109
35	Ab initio chemical potentials of solid and liquid solutions and the chemistry of the Earthâ€™s core. Journal of Chemical Physics, 2002, 116, 7127-7136.	3.0	107
36	Thermal Stability of Corrugated Epitaxial Graphene Grown on Re(0001). Physical Review Letters, 2011, 106, 216101.	7.8	106

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37	First-Principles Modeling of Non-Covalent Interactions in Supramolecular Systems: The Role of Many-Body Effects. Journal of Chemical Theory and Computation, 2012, 8, 4317-4322.	5.3	104
38	Constraints on the composition of the Earth's core from ab initio calculations. Nature, 2000, 405, 172-175.	27.8	100
39	Melting curve of tantalum from first principles. Physical Review B, 2007, 75, .	3.2	99
40	Ab initio molecular dynamics, a simple algorithm for charge extrapolation. Computer Physics Communications, 1999, 118, 31-33.	7.5	98
41	Assessment of density functional theory for iron(II) molecules across the spin-crossover transition. Journal of Chemical Physics, 2012, 137, 124303.	3.0	94
42	First-principles simulations of direct coexistence of solid and liquid aluminum. Physical Review B, 2003, 68, .	3.2	93
43	Physisorption of Water on Graphene: Subchemical Accuracy from Many-Body Electronic Structure Methods. Journal of Physical Chemistry Letters, 2019, 10, 358-368.	4.6	90
44	Ab initio free energy calculations on the polymorphs of iron at core conditions. Physics of the Earth and Planetary Interiors, 2000, 117, 123-137.	1.9	89
45	Ab initiomelting curve of molybdenum by the phase coexistence method. Journal of Chemical Physics, 2007, 126, 194502.	3.0	89
46	Complementary approaches to the ab initio calculation of melting properties. Journal of Chemical Physics, 2002, 116, 6170-6177.	3.0	88
47	First-principles simulations of liquid Fe-S under Earthâ€™s core conditions. Physical Review B, 1998, 58, 8248-8256.	3.2	84
48	Elasticity of CaSiO3 perovskite at high pressure and high temperature. Physics of the Earth and Planetary Interiors, 2006, 155, 249-259.	1.9	84
49	Temperature and composition of the Earth's core. Contemporary Physics, 2007, 48, 63-80.	1.8	84
50	The water-benzene interaction: Insight from electronic structure theories. Journal of Chemical Physics, 2009, 130, 154303.	3.0	73
51	Structural properties and enthalpy of formation of magnesium hydride from quantum Monte Carlo calculations. Physical Review B, 2008, 77, .	3.2	72
52	Extension of molecular electronic structure methods to the solid state: computation of the cohesive energy of lithium hydride. Physical Chemistry Chemical Physics, 2006, 8, 5178.	2.8	70
53	Melting of Iron under Earthâ€™s Core Conditions from Diffusion MonteÂCarlo Free Energy Calculations. Physical Review Letters, 2009, 103, 078501.	7.8	70
54	Theoretical investigation of the high pressure structure, lattice dynamics, phase transition, and thermal equation of state of titanium metal. Journal of Applied Physics, 2010, 107, .	2.5	70

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55	Schottky defect formation energy in MgO calculated by diffusion Monte Carlo. Physical Review B, 2005, 71, .	3.2	69
56	Nanoscale Ï€â€“Ï€ stacked molecules are bound by collective charge fluctuations. Nature Communications, 2017, 8, 14052.	12.8	69
57	Fast and accurate quantum Monte Carlo for molecular crystals. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 1724-1729.	7.1	69
58	Ab initiomelting curve of copper by the phase coexistence approach. Journal of Chemical Physics, 2004, 120, 2872-2878.	3.0	68
59	Development of an electron-temperature-dependent interatomic potential for molecular dynamics simulation of tungsten under electronic excitation. Physical Review B, 2008, 78, .	3.2	68
60	The kinetics of homogeneous melting beyond the limit of superheating. Journal of Chemical Physics, 2011, 135, 024102.	3.0	68
61	First-Principles Simulations of Lithium Melting: Stability of the bcc Phase Close to Melting. Physical Review Letters, 2010, 104, 185701.	7.8	67
62	Calculation of properties of crystalline lithium hydride using correlated wave function theory. Physical Review B, 2009, 80, .	3.2	66
63	Hydrogen dissociation and diffusion on Ni- and Ti-doped Mg(0001) surfaces. Journal of Chemical Physics, 2008, 128, 094703.	3.0	65
64	Iron at Earth's Core Conditions from First Principles Calculations. Reviews in Mineralogy and Geochemistry, 2010, 71, 337-354.	4.8	64
65	Electrical and thermal conductivity of liquid sodium from first-principles calculations. Physical Review B, 2011, 84, .	3.2	64
66	Assessing the accuracy of quantum Monte Carlo and density functional theory for energetics of small water clusters. Journal of Chemical Physics, 2012, 136, 244105.	3.0	64
67	The axial ratio of hcp iron at the conditions of the Earthâ€™s inner core. Physics of the Earth and Planetary Interiors, 2005, 152, 67-77.	1.9	63
68	Proton ordering in cubic ice and hexagonal ice; a potential new ice phaseâ€”XIc. Physical Chemistry Chemical Physics, 2011, 13, 19788.	2.8	60
69	Energy benchmarks for water clusters and ice structures from an embedded many-body expansion. Journal of Chemical Physics, 2013, 139, 114101.	3.0	60
70	Melting curve of materials: theory versus experiments. Journal of Physics Condensed Matter, 2004, 16, S973-S982.	1.8	59
71	First principles calculations on the diffusivity and viscosity of liquid Feâ€“S at experimentally accessible conditions. Physics of the Earth and Planetary Interiors, 2000, 120, 145-152.	1.9	58
72	Quantum Monte Carlo calculations of the structural properties and the B1-B2 phase transition of MgO. Physical Review B, 2005, 72, .	3.2	57

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73	Communication: Water on hexagonal boron nitride from diffusion Monte Carlo. Journal of Chemical Physics, 2015, 142, 181101.	3.0	56
74	Constraints on the phase diagram of molybdenum from first-principles free-energy calculations. Physical Review B, 2012, 85, .	3.2	55
75	Boosting the accuracy and speed of quantum Monte Carlo: Size consistency and time step. Physical Review B, 2016, 93, .	3.2	54
76	Oxygen in the Earth's core: a first-principles study. Physics of the Earth and Planetary Interiors, 1999, 110, 191-210.	1.9	51
77	Direct observation of a dispersionless impurity band in hydrogenated graphene. Physical Review B, 2011, 83, .	3.2	49
78	Local Electronic Structure and Density of Edge and Facet Atoms at Rh Nanoclusters Self-Assembled on a Graphene Template. ACS Nano, 2012, 6, 3034-3043.	14.6	49
79	Binding of hydrogen on benzene, coronene, and graphene from quantum Monte Carlo calculations. Journal of Chemical Physics, 2011, 134, 134701.	3.0	48
80	The structure of iron under the conditions of the Earth's inner core. Geophysical Research Letters, 1999, 26, 1231-1234.	4.0	47
81	Interaction between water and carbon nanostructures: How good are current density functional approximations?. Journal of Chemical Physics, 2019, 151, 164702.	3.0	47
82	Phase stability of CaSiO3 perovskite at high pressure and temperature: Insights from ab initio molecular dynamics. Physics of the Earth and Planetary Interiors, 2006, 155, 260-268.	1.9	46
83	Evidence for stable square ice from quantum Monte Carlo. Physical Review B, 2016, 94, .	3.2	46
84	Fine tuning of graphene-metal adhesion by surface alloying. Scientific Reports, 2013, 3, 2430.	3.3	43
85	Properties of the water to boron nitride interaction: From zero to two dimensions with benchmark accuracy. Journal of Chemical Physics, 2017, 147, 044710.	3.0	43
86	Lattice electrical resistivity of magnetic bcc iron from first-principles calculations. Physical Review B, 2012, 85, .	3.2	42
87	Cooperative Interplay of van der Waals Forces and Quantum Nuclear Effects on Adsorption: H at Graphene and at Coronene. ACS Nano, 2014, 8, 9905-9913.	14.6	42
88	The reconstruction of Rh(001) upon oxygen adsorption. Surface Science, 1998, 410, 151-157.	1.9	41
89	The incorporation of water into lower-mantle perovskites: A first-principles study. Earth and Planetary Science Letters, 2013, 364, 37-43.	4.4	41
90	Benchmarking the performance of density functional theory and point charge force fields in their description of sI methane hydrate against diffusion Monte Carlo. Journal of Chemical Physics, 2014, 140, 174703.	3.0	41

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91	Performance of van der Waals Corrected Functionals for Guest Adsorption in the M₂(dobdc) Metalâ€“Organic Frameworks. Journal of Physical Chemistry A, 2017, 121, 4139-4151.	2.5	41
92	Hydrogen dissociation on Mg(0001) studied via quantum Monte Carlo calculations. Physical Review B, 2008, 78, .	3.2	40
93	Melting curve of face-centered-cubic nickel from first-principles calculations. Physical Review B, 2013, 88, .	3.2	40
94	Phonon Spectroscopy of Oriented hcp Iron. High Pressure Research, 2002, 22, 501-506.	1.2	39
95	Diamond andÎ²-tin structures of Si studied with quantum Monte Carlo calculations. Physical Review B, 2004, 70, .	3.2	39
96	Structural relaxation and low-energy properties of twisted bilayer graphene. Physical Review Research, 2020, 2, .	3.6	39
97	Exchange-correlation energy and the phase diagram of Si. Physical Review B, 2003, 68, .	3.2	38
98	Ab initiothermodynamics and phase diagram of solid magnesium: A comparison of the LDA and GGA. Journal of Chemical Physics, 2006, 125, 194507.	3.0	38
99	Structural and thermodynamic properties of compressed palladium:Ab initioand molecular dynamics study. Physical Review B, 2011, 83, .	3.2	38
100	Ab initio calculation of lattice dynamics and thermodynamic properties of beryllium. Journal of Applied Physics, 2012, 111, .	2.5	38
101	How strongly do hydrogen and water molecules stick to carbon nanomaterials?. Journal of Chemical Physics, 2017, 146, .	3.0	38
102	The energetics of oxide surfaces by quantum Monte Carlo. Journal of Physics Condensed Matter, 2006, 18, L435-L440.	1.8	37
103	Bottom-up approach for the low-cost synthesis of graphene-alumina nanosheet interfaces using bimetallic alloys. Nature Communications, 2014, 5, 5062.	12.8	37
104	The reconstruction of nickel and rhodium (001) surfaces upon carbon, nitrogen or oxygen adsorptions. Surface Science, 1999, 437, 18-28.	1.9	36
105	The particle-in-cell model for ab initio thermodynamics: implications for the elastic anisotropy of the Earthâ€™s inner core. Physics of the Earth and Planetary Interiors, 2003, 139, 243-253.	1.9	36
106	Linear-scaling quantum Monte Carlo technique with non-orthogonal localized orbitals. Journal of Physics Condensed Matter, 2004, 16, L305-L311.	1.8	35
107	A comparison between quantum chemistry and quantum Monte Carlo techniques for the adsorption of water on the (001) LiH surface. Journal of Chemical Physics, 2017, 146, 204108.	3.0	35
108	Thermodynamics from first principles: temperature and composition of the Earthâ€™s core. Mineralogical Magazine, 2003, 67, 113-123.	1.4	34

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109	Elasticity of Mg2SiO4 ringwoodite at mantle conditions. Physics of the Earth and Planetary Interiors, 2006, 157, 181-187.	1.9	34
110	The stability of bcc-Fe at high pressures and temperatures with respect to tetragonal strain. Physics of the Earth and Planetary Interiors, 2008, 170, 52-59.	1.9	34
111	First-principles energetics of water clusters and ice: A many-body analysis. Journal of Chemical Physics, 2013, 139, 244504.	3.0	34
112	HREEL spectra of various oxygen structures on Rh(110). Chemical Physics Letters, 1993, 211, 220-226.	2.6	32
113	The ab initio simulation of the Earth's core. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2002, 360, 1227-1244.	3.4	31
114	Ab initio calculations on the free energy and high Pâ€“T elasticity of face-centred-cubic iron. Earth and Planetary Science Letters, 2008, 268, 444-449.	4.4	31
115	High-temperature behavior of supported graphene: Electron-phonon coupling and substrate-induced doping. Physical Review B, 2012, 86, .	3.2	31
116	Communication: Energy benchmarking with quantum Monte Carlo for water nano-droplets and bulk liquid water. Journal of Chemical Physics, 2013, 138, 221102.	3.0	31
117	Phonon Density of States and Compression Behavior in Iron Sulfide under Pressure. Physical Review Letters, 2004, 93, 195503.	7.8	30
118	Comment on â€œMolybdenum at High Pressure and Temperature: Melting from Another Solid Phaseâ€• Physical Review Letters, 2008, 101, 049601; author reply 049602.	7.8	30
119	Epitaxy of Nanocrystalline Silicon Carbide on Si(111) at Room Temperature. Journal of the American Chemical Society, 2012, 134, 17400-17403.	13.7	30
120	Structural, vibrational and thermodynamic properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si566.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Mg</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si567.gif" overflow="scroll"><mml:mrow><mml:msu. Physics of the Earth and Planetary Interiors, 2015, 240, 1-24.	1.9	30
121	Toward Accurate Adsorption Energetics on Clay Surfaces. Journal of Physical Chemistry C, 2016, 120, 26402-26413.	3.1	30
122	Electrical resistivity of solid and liquid Cu up to 5ÂGPa: Decrease along the melting boundary. Journal of Physics and Chemistry of Solids, 2017, 110, 386-393.	4.0	30
123	Adsorption of a water molecule on the MgO(100) surface as described by cluster and slab models. Physical Chemistry Chemical Physics, 2012, 14, 7846.	2.8	29
124	On core convection and the geodynamo: Effects of high electrical and thermal conductivity. Physics of the Earth and Planetary Interiors, 2015, 247, 56-64.	1.9	29
125	The melting curve of iron from quantum mechanics calculations. Journal of Physics and Chemistry of Solids, 2004, 65, 1573-1580.	4.0	28
126	Equation of state of hexagonal closed packed iron under Earthâ€™s core conditions from quantum Monte Carlo calculations. Physical Review B, 2009, 79, .	3.2	28

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127	Melting temperature of tungsten from twoab initioapproaches. Physical Review B, 2011, 84, .	3.2	28
128	Compositional instability of Earth's solid inner core. Geophysical Research Letters, 2013, 40, 1084-1088.	4.0	28
129	Spin-Flop Ordering from Frustrated Ferro- and Antiferromagnetic Interactions: A Combined Theoretical and Experimental Study of aMn/Fe(100)Monolayer. Physical Review Letters, 2005, 95, 117201.	7.8	27
130	Bulk and surface energetics of crystalline lithium hydride: Benchmarks from quantum Monte Carlo and quantum chemistry. Physical Review B, 2010, 82, .	3.2	27
131	Recent developments in ab initio thermodynamics. , 2000, 77, 871-879.		26
132	Zero-temperature generalized phase diagram of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>4</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>transition metals under pressure. Physical Review B, 2008, 77, .	3.2	26
133	First-principles calculations of elastic and electronic properties of NbB₂under pressure. Journal of Physics Condensed Matter, 2009, 21, 025505.	1.8	26
134	Saturation of electrical resistivity of solid iron at Earthâ€™s core conditions. SpringerPlus, 2016, 5, 256.	1.2	26
135	Highâ€precision calculation of Hartreeâ€Fock energy of crystals. Journal of Computational Chemistry, 2008, 29, 2098-2106.	3.3	25
136	Ab initiocalculations of the thermodynamics and phase diagram of zirconium. Physical Review B, 2008, 78, .	3.2	25
137	Including the effects of pressure and stress in thermodynamic functions. Physica Status Solidi (B): Basic Research, 2014, 251, 81-96.	1.5	25
138	Water on BN doped benzene: A hard test for exchange-correlation functionals and the impact of exact exchange on weak binding. Journal of Chemical Physics, 2014, 141, 18C530.	3.0	25
139	Communication: On the stability of ice 0, ice i, and Ih. Journal of Chemical Physics, 2014, 141, 161102.	3.0	25
140	Nuclear quantum effects on the high pressure melting of dense lithium. Journal of Chemical Physics, 2015, 142, 064506.	3.0	25
141	A new scheme for fixed node diffusion quantum Monte Carlo with pseudopotentials: Improving reproducibility and reducing the trial-wave-function bias. Journal of Chemical Physics, 2019, 151, 134105.	3.0	25
142	Ab initio molecular dynamics simulations for thermal equation of state of B2-type NaCl. Journal of Applied Physics, 2008, 103, 023510.	2.5	24
143	Structure and elasticity of hydrous ringwoodite: A first principle investigation. Physics of the Earth and Planetary Interiors, 2009, 177, 103-115.	1.9	23
144	The competition for graphene formation on Re(0001): A complex interplay between carbon segregation, dissolution and carburisation. Carbon, 2014, 73, 389-402.	10.3	23

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145	Carbon Partitioning Between the Earth's Inner and Outer Core. Journal of Geophysical Research: Solid Earth, 2019, 124, 12812-12824.	3.4	23
146	Partitioning of sulfur between solid and liquid iron under Earthâ€™s core conditions: Constraints from atomistic simulations with machine learning potentials. Geochimica Et Cosmochimica Acta, 2020, 291, 5-18.	3.9	23
147	Pandemic drugs at pandemic speed: infrastructure for accelerating COVID-19 drug discovery with hybrid machine learning- and physics-based simulations on high-performance computers. Interface Focus, 2021, 11, 20210018.	3.0	23
148	Ab initio statistical mechanics of surface adsorption and desorption. I. H2O on MgO (001) at low coverage. Journal of Chemical Physics, 2007, 127, 114709.	3.0	20
149	Ab initio lattice dynamics calculations on the combined effect of temperature and silicon on the stability of different iron phases in the Earth's inner core. Physics of the Earth and Planetary Interiors, 2010, 178, 2-7.	1.9	20
150	Tuning dissociation using isoelectronically doped graphene and hexagonal boron nitride: Water and other small molecules. Journal of Chemical Physics, 2016, 144, 154706.	3.0	20
151	Electronic correlations and transport in iron at Earthâ€™s core conditions. Nature Communications, 2020, 11, 4105.	12.8	20
152	On the room-temperature phase diagram of high pressure hydrogen: An ab initio molecular dynamics perspective and a diffusion Monte Carlo study. Journal of Chemical Physics, 2014, 141, 024501.	3.0	19
153	Unravelling the roles of surface chemical composition and geometry for the grapheneâ€“metal interaction through C1s core-level spectroscopy. Carbon, 2015, 93, 187-198.	10.3	18
154	Thermodynamic Stability of Fe/O Solid Solution at Inner-Core Conditions. Geophysical Research Letters, 2000, 27, 2417-2420.	4.0	17
155	The role of steps in the dissociation of H₂on Mg(0001). Journal of Physics Condensed Matter, 2009, 21, 095004.	1.8	17
156	Assessing the inner core nucleation paradox with atomic-scale simulations. Earth and Planetary Science Letters, 2019, 507, 1-9.	4.4	17
157	Ground state of a spin-crossover molecule calculated by diffusion Monte Carlo. Physical Review B, 2013, 87, .	3.2	16
158	Analyzing the errors of DFT approximations for compressed water systems. Journal of Chemical Physics, 2014, 141, 014104.	3.0	16
159	Absolute rate of thermal desorption from first-principles simulation. Journal of Physics Condensed Matter, 2006, 18, L451-L457.	1.8	15
160	Melting properties of a simple tight-binding model of transition metals. I. The region of half-filled d-band. Journal of Chemical Physics, 2009, 130, 174707.	3.0	15
161	A new belt-type apparatus for neutron-based rheological measurements at gigapascal pressures. High Pressure Research, 2005, 25, 107-118.	1.2	14
162	Ab initio molecular dynamics study of elasticity of akimotoite MgSiO3 at mantle conditions. Physics of the Earth and Planetary Interiors, 2009, 173, 115-120.	1.9	14

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163	Structure, hydrogen bonding and thermal expansion of ammonium carbonate monohydrate. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2014, 70, 948-962.	1.1	14
164	Energy benchmarks for methane-water systems from quantum Monte Carlo and second-order MÃ¸ller-Plesset calculations. Journal of Chemical Physics, 2015, 143, 102812.	3.0	14
165	Ab initio molecular dynamic simulation on the elasticity of Mg3Al2Si3O12 pyrope. Journal of Earth Science (Wuhan, China), 2011, 22, 169-175.	3.2	13
166	Transfer of oxygen to Earth's core from a long-lived magma ocean. Earth and Planetary Science Letters, 2020, 538, 116208.	4.4	13
167	Ab-initiosimulations of magnetic iron sulphides. Molecular Simulation, 2005, 31, 379-384.	2.0	12
168	Non-adiabatic ab initio molecular dynamics of supersonic beam epitaxy of silicon carbide at room temperature. Journal of Chemical Physics, 2013, 138, 044701.	3.0	12
169	Molecular Lifting, Twisting, and Curling during Metal-Assisted Polycyclic Hydrocarbon Dehydrogenation. Journal of the American Chemical Society, 2016, 138, 3395-3402.	13.7	12
170	Partitioning of Oxygen Between Ferropericlase and Earth's Liquid Core. Geophysical Research Letters, 2018, 45, 6042-6050.	4.0	12
171	Phonon Softening and Elastic Instabilities in the Cubic-to-Orthorhombic Structural Transition of CsH. Physical Review Letters, 1997, 78, 4958-4961.	7.8	11
172	Transport coefficients of liquids from first principles. Journal of Non-Crystalline Solids, 1999, 250-252, 82-90.	3.1	11
173	Melting curve and Hugoniot of molybdenum up to 400 GPa byab initiosimulations. Journal of Physics: Conference Series, 2008, 121, 012009.	0.4	11
174	Benchmarking DFT surface energies with quantum Monte Carlo. Molecular Simulation, 2009, 35, 609-612.	2.0	11
175	Translucency of Graphene to van der Waals Forces Applies to Atoms/Molecules with Different Polar Character. ACS Nano, 2019, 13, 12230-12241.	14.6	11
176	Pressure-induced amorphization of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Cu</mml:mi><mml:mi mathvariant="normal">Fe</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>studied by<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mmultiscripts><mml:mi mathvariant="normal">Fe</mml:mi><mml:mprescripts />	3.2	10
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