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	Thermodynamic and structural insights into the repurposing of drugs that bind to SARS-CoV-2 main protease. Molecular Systems Design and Engineering, 2022, 7, 123-131.	3.4	5
2	Materials and Molecular Modeling at the Exascale. Computing in Science and Engineering, 2022, 24, 36-45.	1.2	7
3	Towards reconciling experimental and computational determinations of Earth's core thermal conductivity. Earth and Planetary Science Letters, 2022, 584, 117466.	4.4	10
4	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>B</mml:mi><mml:mn>1</mml:mn><mml:mtext>â</mml:mtext><mml:mo>ˆ</mml:mo><mml:mtext>’</mml:mtext></mml:mrow></mml:math> phase transition of ferropericlase at planetary interior conditions. Physical Review B, 2022, 105, .	3.2	2
5	Unusual reversibility in molecular break-up of PAHs: the case of pentacene dehydrogenation on Ir(111). Chemical Science, 2021, 12, 170-178.	7.4	4
6	Atomic Undercoordination in Ag Islands on Ru(0001) Grown via Size-Selected Cluster Deposition: An Experimental and Theoretical High-Resolution Core-Level Photoemission Study. Journal of Physical Chemistry C, 2021, 125, 9556-9563.	3.1	4
7	Molecular dynamics study of the point defects in bcc uranium. Physical Review Materials, 2021, 5, .	2.4	2
8	Probing the nucleation of iron in Earth's core using molecular dynamics simulations of supercooled liquids. Physical Review B, 2021, 103, .	3.2	4
9	Melting line of calcium characterized by in situ LH-DAC XRD and first-principles calculations. Scientific Reports, 2021, 11, 15025.	3.3	2
10	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
11	Enhancing the Accuracy of Ab Initio Molecular Dynamics by Fine Tuning of Effective Two-Body Interactions: Acetonitrile as a Test Case. Journal of Physical Chemistry A, 2021, 125, 10475-10484.	2.5	4
12	Interfacial two-dimensional oxide enhances photocatalytic activity of graphene/titania via electronic structure modification. Carbon, 2020, 157, 350-357.	10.3	7
13	Electronic correlations and transport in iron at Earthâ€™s core conditions. Nature Communications, 2020, 11, 4105.	12.8	20
14	Transfer of oxygen to Earth's core from a long-lived magma ocean. Earth and Planetary Science Letters, 2020, 538, 116208.	4.4	13
15	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
16	Structural relaxation and low-energy properties of twisted bilayer graphene. Physical Review Research, 2020, 2, .	3.6	39
17	Structure of graphene and a surface carbide grown on the (0001) surface of rhenium. Physical Review Materials, 2020, 4, .	2.4	0
18	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

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19	FeO Content of Earthâ€™s Liquid Core. Physical Review X, 2019, 9, .	8.9	7
20	Interaction between water and carbon nanostructures: How good are current density functional approximations?. Journal of Chemical Physics, 2019, 151, 164702.	3.0	47
21	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
22	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
23	Carbon Partitioning Between the Earth's Inner and Outer Core. Journal of Geophysical Research: Solid Earth, 2019, 124, 12812-12824.	3.4	23
24	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
25	Assessing the inner core nucleation paradox with atomic-scale simulations. Earth and Planetary Science Letters, 2019, 507, 1-9.	4.4	17
26	Development of a machine learning potential for graphene. Physical Review B, 2018, 97, .	3.2	142
27	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
28	Mg partitioning between solid and liquid iron under the Earthâ€™s core conditions. Physics of the Earth and Planetary Interiors, 2018, 274, 218-221.	1.9	8
29	Partitioning of Oxygen Between Ferropericlase and Earth's Liquid Core. Geophysical Research Letters, 2018, 45, 6042-6050.	4.0	12
30	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
31	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
32	How strongly do hydrogen and water molecules stick to carbon nanomaterials?. Journal of Chemical Physics, 2017, 146, .	3.0	38
33	Nanoscale Ï€â€“Ï€ stacked molecules are bound by collective charge fluctuations. Nature Communications, 2017, 8, 14052.	12.8	69
34	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
35	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
36	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

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37	Perspective: How good is DFT for water?. Journal of Chemical Physics, 2016, 144, 130901.	3.0	571
38	Evidence for stable square ice from quantum Monte Carlo. Physical Review B, 2016, 94, .	3.2	46
39	Boosting the accuracy and speed of quantum Monte Carlo: Size consistency and time step. Physical Review B, 2016, 93, .	3.2	54
40	Toward Accurate Adsorption Energetics on Clay Surfaces. Journal of Physical Chemistry C, 2016, 120, 26402-26413.	3.1	30
41	Saturation of electrical resistivity of solid iron at Earthâ€™s core conditions. SpringerPlus, 2016, 5, 256.	1.2	26
42	Molecular Lifting, Twisting, and Curling during Metal-Assisted Polycyclic Hydrocarbon Dehydrogenation. Journal of the American Chemical Society, 2016, 138, 3395-3402.	13.7	12
43	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
44	Structure of magnesium selenate enneahydrate, MgSeO4Â·9H2O, from 5 to 250â€…K using neutron time-of-flight Laue diffraction. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2015, 71, 313-327.	1.1	4
45	Elasticity, anelasticity 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> 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
46	Comparison of polynomial approximations to speed up planewave-based quantum Monte Carlo calculations. Journal of Computational Physics, 2015, 287, 77-87.	3.8	2
47	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
48	The Ab Initio Treatment of High-Pressure and High-Temperature Mineral Properties and Behavior. , 2015, , 369-392.		2
49	Nuclear quantum effects on the high pressure melting of dense lithium. Journal of Chemical Physics, 2015, 142, 064506.	3.0	25
50	Communication: Water on hexagonal boron nitride from diffusion Monte Carlo. Journal of Chemical Physics, 2015, 142, 181101.	3.0	56
51	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
52	Constraints from material properties on the dynamics and evolution of Earthâ€™s core. Nature Geoscience, 2015, 8, 678-685.	12.9	117
53	Anharmonicity, mechanical instability, and thermodynamic properties of the Cr-Re Ïƒ-phase. Journal of Chemical Physics, 2014, 140, 144502.	3.0	6
54	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

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55	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
56	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
57	Including the effects of pressure and stress in thermodynamic functions. Physica Status Solidi (B): Basic Research, 2014, 251, 81-96.	1.5	25
58	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
59	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
60	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
61	Communication: On the stability of ice 0, ice i, and Ih. Journal of Chemical Physics, 2014, 141, 161102.	3.0	25
62	Analyzing the errors of DFT approximations for compressed water systems. Journal of Chemical Physics, 2014, 141, 014104.	3.0	16
63	Hard Numbers for Large Molecules: Toward Exact Energetics for Supramolecular Systems. Journal of Physical Chemistry Letters, 2014, 5, 849-855.	4.6	159
64	Bottom-up approach for the low-cost synthesis of graphene-alumina nanosheet interfaces using bimetallic alloys. Nature Communications, 2014, 5, 5062.	12.8	37
65	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
66	Melting curve of face-centered-cubic nickel from first-principles calculations. Physical Review B, 2013, 88, .	3.2	40
67	First-principles energetics of water clusters and ice: A many-body analysis. Journal of Chemical Physics, 2013, 139, 244504.	3.0	34
68	Fine tuning of graphene-metal adhesion by surface alloying. Scientific Reports, 2013, 3, 2430.	3.3	43
69	The incorporation of water into lower-mantle perovskites: A first-principles study. Earth and Planetary Science Letters, 2013, 364, 37-43.	4.4	41
70	Energy benchmarks for water clusters and ice structures from an embedded many-body expansion. Journal of Chemical Physics, 2013, 139, 114101.	3.0	60
71	Ground state of a spin-crossover molecule calculated by diffusion Monte Carlo. Physical Review B, 2013, 87, .	3.2	16
72	Transport properties for liquid silicon-oxygen-iron mixtures at Earth's core conditions. Physical Review B, 2013, 87, .	3.2	131

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73	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
74	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
75	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
76	Compositional instability of Earth's solid inner core. Geophysical Research Letters, 2013, 40, 1084-1088.	4.0	28
77	Ab initio calculation of lattice dynamics and thermodynamic properties of beryllium. Journal of Applied Physics, 2012, 111, .	2.5	38
78	High-temperature behavior of supported graphene: Electron-phonon coupling and substrate-induced doping. Physical Review B, 2012, 86, .	3.2	31
79	Lattice electrical resistivity of magnetic bcc iron from first-principles calculations. Physical Review B, 2012, 85, .	3.2	42
80	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
81	Non-local Effects on Oxygen-Induced Surface Core Level Shifts of Re(0001). Journal of Physical Chemistry C, 2012, 116, 23297-23307.	3.1	10
82	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
83	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
84	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
85	Epitaxy of Nanocrystalline Silicon Carbide on Si(111) at Room Temperature. Journal of the American Chemical Society, 2012, 134, 17400-17403.	13.7	30
86	Thermal and electrical conductivity of iron at Earthâ€™s core conditions. Nature, 2012, 485, 355-358.	27.8	510
87	Assessment of density functional theory for iron(II) molecules across the spin-crossover transition. Journal of Chemical Physics, 2012, 137, 124303.	3.0	94
88	Constraints on the phase diagram of molybdenum from first-principles free-energy calculations. Physical Review B, 2012, 85, .	3.2	55
89	Hydrogen Concentration Estimation Based on Density Functional Theory in Aluminum and Alpha Iron under Gaseous Hydrogen Environments. Transactions of the Materials Research Society of Japan, 2012, 37, 1-6.	0.2	5
90	Thermal Stability of Corrugated Epitaxial Graphene Grown on Re(0001). Physical Review Letters, 2011, 106, 216101.	7.8	106

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91	Proton ordering in cubic ice and hexagonal ice; a potential new ice phaseâ€"XIc. Physical Chemistry Chemical Physics, 2011, 13, 19788.	2.8	60
92	Hydrogen Bonds and van der Waals Forces in Ice at Ambient and High Pressures. Physical Review Letters, 2011, 107, 185701.	7.8	193
93	Binding of hydrogen on benzene, coronene, and graphene from quantum Monte Carlo calculations. Journal of Chemical Physics, 2011, 134, 134701.	3.0	48
94	Thermal Expansion of Supported and Freestanding Graphene: Lattice Constant versus Interatomic Distance. Physical Review Letters, 2011, 106, 135501.	7.8	148
95	Adsorption and diffusion of water on graphene from first principles. Physical Review B, 2011, 84, .	3.2	218
96	A simple tight-binding model for the study of 4d transition metals under pressure. Computational Materials Science, 2011, 50, 2732-2735.	3.0	3
97	Prospecting for water in the transition zone: d ln(Vs)/d ln(Vp). Physics of the Earth and Planetary Interiors, 2011, 189, 117-120.	1.9	9
98	The kinetics of homogeneous melting beyond the limit of superheating. Journal of Chemical Physics, 2011, 135, 024102.	3.0	68
99	Electrical and thermal conductivity of liquid sodium from first-principles calculations. Physical Review B, 2011, 84, .	3.2	64
100	Dehydrogenation of pure and Ti-doped Na3AlH6 surfaces from first principles calculations. International Journal of Hydrogen Energy, 2011, 36, 15632-15641.	7.1	8
101	Melting temperature of tungsten from twoab initioapproaches. Physical Review B, 2011, 84, .	3.2	28
102	Ab initio molecular dynamic simulation on the elasticity of Mg3Al2Si3O12 pyrope. Journal of Earth Science (Wuhan, China), 2011, 22, 169-175.	3.2	13
103	Structural and thermodynamic properties of compressed palladium:Ab initioand molecular dynamics study. Physical Review B, 2011, 83, .	3.2	38
104	Direct observation of a dispersionless impurity band in hydrogenated graphene. Physical Review B, 2011, 83, .	3.2	49
105	16. Iron at Earth's Core Conditions from First Principles Calculations. , 2010, , 337-354.		0
106	Iron at Earth's Core Conditions from First Principles Calculations. Reviews in Mineralogy and Geochemistry, 2010, 71, 337-354.	4.8	64
107	Ab initio statistical mechanics of surface adsorption and desorption. II. Nuclear quantum effects. Journal of Chemical Physics, 2010, 133, 044103.	3.0	10
108	First-Principles Simulations of Lithium Melting: Stability of the bcc Phase Close to Melting. Physical Review Letters, 2010, 104, 185701.	7.8	67

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109	Determining the Chemical Reactivity Trends of Pd/Ru(0001) Pseudomorphic Overlayers: Core-Level Shift Measurements and DFT Calculations. Journal of Physical Chemistry C, 2010, 114, 436-441.	3.1	5
110	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
111	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
112	Bulk and surface energetics of crystalline lithium hydride: Benchmarks from quantum Monte Carlo and quantum chemistry. Physical Review B, 2010, 82, .	3.2	27
113	Calculation of properties of crystalline lithium hydride using correlated wave function theory. Physical Review B, 2009, 80, .	3.2	66
114	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
115	Publisherâ€™s Note: Growth of Dome-Shaped Carbon Nanoislands on Ir(111): The Intermediate between Carbidic Clusters and Quasi-Free-Standing Graphene [Phys. Rev. Lett.103, 166101 (2009)]. Physical Review Letters, 2009, 103, .	7.8	4
116	Melting of Iron under Earthâ€™s Core Conditions from Diffusion MonteÂCarlo Free Energy Calculations. Physical Review Letters, 2009, 103, 078501.	7.8	70
117	Benchmarking DFT surface energies with quantum Monte Carlo. Molecular Simulation, 2009, 35, 609-612.	2.0	11
118	First-principles calculations of elastic and electronic properties of NbB₂under pressure. Journal of Physics Condensed Matter, 2009, 21, 025505.	1.8	26
119	The role of steps in the dissociation of H₂on Mg(0001). Journal of Physics Condensed Matter, 2009, 21, 095004.	1.8	17
120	PHON: A program to calculate phonons using the small displacement method. Computer Physics Communications, 2009, 180, 2622-2633.	7.5	664
121	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
122	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
123	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
124	Structure and elasticity of hydrous ringwoodite: A first principle investigation. Physics of the Earth and Planetary Interiors, 2009, 177, 103-115.	1.9	23
125	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
126	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

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127	The water-benzene interaction: Insight from electronic structure theories. Journal of Chemical Physics, 2009, 130, 154303.	3.0	73
128	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
129	Highâ€precision calculation of Hartreeâ€Fock energy of crystals. Journal of Computational Chemistry, 2008, 29, 2098-2106.	3.3	25
130	Structural properties and enthalpy of formation of magnesium hydride from quantum Monte Carlo calculations. Physical Review B, 2008, 77, .	3.2	72
131	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
132	Hydrogen dissociation and diffusion on Ni- and Ti-doped Mg(0001) surfaces. Journal of Chemical Physics, 2008, 128, 094703.	3.0	65
133	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
134	Ab initiocalculations of the thermodynamics and phase diagram of zirconium. Physical Review B, 2008, 78, .	3.2	25
135	Melting curve and Hugoniot of molybdenum up to 400 GPa byab initiosimulations. Journal of Physics: Conference Series, 2008, 121, 012009.	0.4	11
136	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
137	Ab initio molecular dynamics simulations for thermal equation of state of B2-type NaCl. Journal of Applied Physics, 2008, 103, 023510.	2.5	24
138	Effect of the exchange-correlation energy and temperature on the generalized phase diagram of the 4dtransition metals. High Pressure Research, 2008, 28, 449-453.	1.2	2
139	Ab-initio melting curve and principal Hugoniot of tantalum. Journal of Physics: Conference Series, 2008, 121, 012010.	0.4	4
140	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
141	Hydrogen dissociation on Mg(0001) studied via quantum Monte Carlo calculations. Physical Review B, 2008, 78, .	3.2	40
142	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
143	Theory and Practice â€“ The Ab Initio Treatment of High-Pressure and -Temperature Mineral Properties and Behavior. , 2007, , 359-387.		1
144	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

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145	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
146	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
147	Ab initiomelting curve of molybdenum by the phase coexistence method. Journal of Chemical Physics, 2007, 126, 194502.	3.0	89
148	Temperature and composition of the Earth's core. Contemporary Physics, 2007, 48, 63-80.	1.8	84
149	Melting curve of tantalum from first principles. Physical Review B, 2007, 75, .	3.2	99
150	Properties and Evolution of the Earth's Core and Geodynamo. Series on Iraq War and Its Consequences, 2007, , 167-209.	0.1	0
151	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
152	Ab initio study of the phase separation of argon in molten iron at high pressures. Geophysical Research Letters, 2006, 33, .	4.0	8
153	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
154	Elasticity of CaSiO3 perovskite at high pressure and high temperature. Physics of the Earth and Planetary Interiors, 2006, 155, 249-259.	1.9	84
155	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
156	Elasticity of Mg2SiO4 ringwoodite at mantle conditions. Physics of the Earth and Planetary Interiors, 2006, 157, 181-187.	1.9	34
157	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
158	The energetics of oxide surfaces by quantum Monte Carlo. Journal of Physics Condensed Matter, 2006, 18, L435-L440.	1.8	37
159	Absolute rate of thermal desorption from first-principles simulation. Journal of Physics Condensed Matter, 2006, 18, L451-L457.	1.8	15
160	Melting Curve of MgO from First-Principles Simulations. Physical Review Letters, 2005, 94, 235701.	7.8	158
161	Schottky defect formation energy in MgO calculated by diffusion Monte Carlo. Physical Review B, 2005, 71, .	3.2	69
162	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

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163	A new belt-type apparatus for neutron-based rheological measurements at gigapascal pressures. High Pressure Research, 2005, 25, 107-118.	1.2	14
164	Ab-initiosimulations of magnetic iron sulphides. Molecular Simulation, 2005, 31, 379-384.	2.0	12
165	Quantum Monte Carlo calculations of the structural properties and the B1-B2 phase transition of MgO. Physical Review B, 2005, 72, .	3.2	57
166	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
167	Linear-scaling quantum Monte Carlo technique with non-orthogonal localized orbitals. Journal of Physics Condensed Matter, 2004, 16, L305-L311.	1.8	35
168	Ab initiomelting curve of copper by the phase coexistence approach. Journal of Chemical Physics, 2004, 120, 2872-2878.	3.0	68
169	An ab initio study of the relative stabilities and equations of state of Fe3S polymorphs. Mineralogical Magazine, 2004, 68, 813-817.	1.4	6
170	Efficient localized basis set for quantum Monte Carlo calculations on condensed matter. Physical Review B, 2004, 70, .	3.2	122
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