Simon R Phillpot

List of Publications by Year in descending order

185 papers	13,991 citations	46984 47 h-index	20943 115 g-index
188 all docs	188 docs citations	188 times ranked	12554 citing authors

#	Article	IF	Citations
1	Nanoscale thermal transport. Journal of Applied Physics, 2003, 93, 793-818.	1.1	2,519
2	Comparison of atomic-level simulation methods for computing thermal conductivity. Physical Review B, 2002, 65, .	1.1	1,315
3	Nanoscale thermal transport. II. 2003â€“2012. Applied Physics Reviews, 2014, 1, 011305.	5.5	1,277
4	Thermal barrier coating materials. Materials Today, 2005, 8, 22-29.	8.3	869
5	Dislocation processes in the deformation of nanocrystalline aluminium by molecular-dynamics simulation. Nature Materials, 2002, 1, 45-49.	13.3	865
6	Low thermal conductivity oxides. MRS Bulletin, 2012, 37, 917-922.	1.7	298
7	Parametrization of a reactive many-body potential for Moâ€“S systems. Physical Review B, 2009, 79, .	1.1	241
8	Classical atomistic simulations of surfaces and heterogeneous interfaces with the charge-optimized many body (COMB) potentials. Materials Science and Engineering Reports, 2013, 74, 255-279.	14.8	222
9	Reactive Potentials for Advanced Atomistic Simulations. Annual Review of Materials Research, 2013, 43, 109-129.	4.3	184
10	Scaling Behavior of Grain-Rotation-Induced Grain Growth. Physical Review Letters, 2002, 89, 206101.	2.9	178
11	Charge optimized many-body potential for theSiâ•SiO2system. Physical Review B, 2007, 75, .	1.1	159
12	Mixed Bloch-NÃ©el-Ising character of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>180</mml:mn><mml:mo>Â°</mml:mo></mml:mrow></mml:math>ferroelectric domain walls. Physical Review B, 2009, 80, .	1.1	146
13	Thermal transport and grain boundary conductance in ultrananocrystalline diamond thin films. Journal of Applied Physics, 2006, 99, 114301.	1.1	139
14	Mechanism of the Cubicâ€“toâ€“Tetragonal Phase Transition in Zirconia and Yttriaâ€Stabilized Zirconia by Molecularâ€Dynamics Simulation. Journal of the American Ceramic Society, 2001, 84, 1609-1619.	1.9	136
15	Mechanism of Thermal Transport in Zirconia and Yttriaâ€Stabilized Zirconia by Molecularâ€Dynamics Simulation. Journal of the American Ceramic Society, 2001, 84, 2997-3007.	1.9	134
16	Phonon Lifetime Investigation of Anharmonicity and Thermal Conductivity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>UO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>by Neutron Scattering and Theory. Physical Review Letters, 2013, 110, 157401.	2.9	132
17	Charge-optimized many-body potential for the hafnium/hafnium oxide system. Physical Review B, 2010, 81, .	1.1	130
18	Energetics of intrinsic point defects in uranium dioxide from electronic-structure calculations. Journal of Nuclear Materials, 2009, 384, 61-69.	1.3	127

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19	Atomic-level simulation of ferroelectricity in oxide materials. Current Opinion in Solid State and Materials Science, 2005, 9, 107-113.	5.6	109
20	Stability of intrinsic defects and defect clusters in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Li</mml:mi><mml:mi mathvariant="normal">Nb</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>from density functional theory calculations. Physical Review B, 2008, 78, .	1.1	109
21	Band gap and structure of single crystal BiI3: Resolving discrepancies in literature. Journal of Applied Physics, 2013, 114, .	1.1	109
22	Atomic-Scale Mechanism of Crack-Tip Plasticity: Dislocation Nucleation and Crack-Tip Shielding. Physical Review Letters, 1997, 79, 1309-1312.	2.9	107
23	First-principles determination of slide potential energy surfaces for atomic friction in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Mo</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Mo</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn	1.1	106
24	Vibrations and thermal transport in nanocrystalline silicon. Physical Review B, 2006, 74, .	1.1	102
25	Hierarchical Materials as Tailored Nuclear Waste Forms: A Perspective. Chemistry of Materials, 2018, 30, 4475-4488.	3.2	98
26	Uncertainty Quantification in Multiscale Simulation of Materials: A Prospective. Annual Review of Materials Research, 2013, 43, 157-182.	4.3	94
27	Variable Charge Reactive Potential for Hydrocarbons to Simulate Organic-Copper Interactions. Journal of Physical Chemistry A, 2012, 116, 7976-7991.	1.1	91
28	Second-generation charge-optimized many-body potential for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Si</mml:mtext><mml:mo>/</mml:mo><mml:msub><mml:mrow><mml:mtext>SiO</mml:mt amorphous silica. Physical Review B, 2010, 82, .	1.1	90
29	Thermal transport properties of uranium dioxide by molecular dynamics simulations. Journal of Nuclear Materials, 2008, 375, 388-396.	1.3	87
30	Grain Boundaries in Uranium Dioxide: Scanning Electron Microscopy Experiments and Atomistic Simulations. Journal of the American Ceramic Society, 2011, 94, 1893-1900.	1.9	78
31	Transition from Thermal to Athermal Friction under Cryogenic Conditions. Physical Review Letters, 2009, 102, 186102.	2.9	73
32	On the Thermodynamic Stability of Amorphous Intergranular Films in Covalent Materials. Journal of the American Ceramic Society, 1997, 80, 717-732.	1.9	72
33	Thermodynamics and Electronic Properties of Heterometallic Multinuclear Actinide-Containing Metalâ€“Organic Frameworks with â€œStructural Memoryâ€. Journal of the American Chemical Society, 2019, 141, 11628-11640.	6.6	71
34	Evaluation of computational techniques for solving the Boltzmann transport equation for lattice thermal conductivity calculations. Physical Review B, 2010, 82, .	1.1	69
35	Atomistic Simulations of Materials Fracture and the Link between Atomic and Continuum Length Scales. Journal of the American Ceramic Society, 1998, 81, 501-516.	1.9	68
36	Atomistic simulations of copper oxidation and Cu/Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O interfaces using charge-optimized many-body potentials. Physical Review B, 2011, 84, .	1.1	68

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37	Phonon Transport Simulator (PhonTS). Computer Physics Communications, 2015, 192, 196-204.	3.0	64
38	Entropy contributions to phase stability in binary random solid solutions. Npj Computational Materials, 2018, 4, .	3.5	64
39	Variable charge many-body interatomic potentials. MRS Bulletin, 2012, 37, 504-512.	1.7	58
40	Thermal Conductivity in Nanocrystalline Ceria Thin Films. Journal of the American Ceramic Society, 2014, 97, 562-569.	1.9	58
41	Mechanistic materials modeling for nuclear fuel performance. Annals of Nuclear Energy, 2017, 105, 11-24.	0.9	57
42	Energetics of Oxidation in MoS₂Nanoparticles by Density Functional Theory. Journal of Physical Chemistry C, 2011, 115, 10606-10616.	1.5	55
43	Sliding orientation effects on the tribological properties of polytetrafluoroethylene. Journal of Applied Physics, 2007, 102, .	1.1	54
44	Nanoindentation of gold and gold alloys by molecular dynamics simulation. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2016, 651, 346-357.	2.6	54
45	Heterometallic Actinideâ€Containing Photoresponsive Metalâ€Organic Frameworks: Dynamic and Static Tuning of Electronic Properties. Angewandte Chemie - International Edition, 2021, 60, 8072-8080.	7.2	51
46	Structure and energetics of 180Â° domain walls in PbTiO₃by density functional theory. Journal of Physics Condensed Matter, 2011, 23, 175902.	0.7	48
47	Critical assessment of UO2 classical potentials for thermal conductivity calculations. Journal of Materials Science, 2012, 47, 7693-7702.	1.7	48
48	Thermal conductance across grain boundaries in diamond from molecular dynamics simulation. Journal of Applied Physics, 2007, 102, 063503.	1.1	47
49	Thermal Transport in Offâ€Stoichiometric Uranium Dioxide by Atomic Level Simulation. Journal of the American Ceramic Society, 2009, 92, 850-856.	1.9	47
50	Molecular dynamics study of the adhesion of Cu/SiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>interfaces using a variable-charge interatomic potential. Physical Review B, 2011, 83, .	1.1	47
51	Vacancyâ€Ordered Structure of Cubic Bismuth Oxide from Simulation and Crystallographic Analysis. Journal of the American Ceramic Society, 2008, 91, 2349-2356.	1.9	45
52	Structure and energetics of ferroelectric domain walls in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LiNbO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml: atomic-level simulations. Physical Review B, 2010, 82, .	1.1	45
53	Phonon density of states and anharmonicity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>UO</mml:mi><mml:mn>2</mml:mn></mml:msub></m Physical Review B, 2014, 89, .	1.1	45
54	Fitting empirical potentials: Challenges and methodologies. Current Opinion in Solid State and Materials Science, 2013, 17, 263-270.	5.6	44

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55	Effects of edge dislocations on thermal transport in UO2. Journal of Nuclear Materials, 2013, 434, 203-209.	1.3	44
56	Crossover in thermal transport properties of natural, perovskite-structured superlattices. Applied Physics Letters, 2009, 95, .	1.5	42
57	A critical assessment of interatomic potentials for ceria with application to its elastic properties. Solid State Ionics, 2010, 181, 551-556.	1.3	42
58	Stability and charge transfer levels of extrinsic defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LiNbO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:r Physical Review B, 2010, 82, .	1.1	41
59	Kinetically evolving irradiation-induced point defect clusters in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>UO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:m molecular dynamics simulation. Physical Review B, 2009, 80, .	1.1	40
60	Thermal transport in polyethylene and at polyethyleneâ€“diamond interfaces investigated using molecular dynamics simulation. Journal of Physics Condensed Matter, 2009, 21, 084219.	0.7	40
61	Atomistic study of grain boundary sink strength under prolonged electron irradiation. Journal of Nuclear Materials, 2012, 422, 69-76.	1.3	40
62	Structure and diffusion of intrinsic defect complexes in LiNbO₃from density functional theory calculations. Journal of Physics Condensed Matter, 2010, 22, 135002.	0.7	39
63	Molecular dynamics investigation of the lubrication mechanism of carbon nano-onions. Computational Materials Science, 2012, 54, 91-96.	1.4	39
64	Effect of Temperature on the Friction and Wear of PTFE by Atomic-Level Simulation. Tribology Letters, 2015, 58, 1.	1.2	38
65	Grapheneâ€“Titanium Interfaces from Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2017, 9, 33288-33297.	4.0	37
66	Structure and energetics of Er defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LiNbO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:r first-principles and thermodynamic calculations. Physical Review B, 2009, 80, .	1.1	35
67	Homogeneous hydride formation path in Î±-Zr: Molecular dynamics simulations with the charge-optimized many-body potential. Acta Materialia, 2016, 111, 357-365.	3.8	35
68	Simulating Multifunctional Structures. Science, 2009, 325, 1634-1635.	6.0	34
69	Effect of the sliding orientation on the tribological properties of polyethylene in molecular dynamics simulations. Journal of Applied Physics, 2008, 103, 083502.	1.1	33
70	Stoichiometry of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">LaFeO</mml:mi><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>(01 surface determined from first-principles and thermodynamic calculations. Physical Review B, 2011, 83, .	1.1	33
71	Microtubule nanospool formation by active self-assembly is not initiated by thermal activation. Soft Matter, 2011, 7, 3108-3115.	1.2	33
72	Molecular dynamics simulation of the shock response of materials: A tutorial. Journal of Applied Physics, 2022, 131, .	1.1	32

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73	Effects of Atomic-Level Disorder at Solid Interfaces. MRS Bulletin, 1990, 15, 38-45.	1.7	31
74	NSF cyberinfrastructures: A new paradigm for advancing materials simulation. Current Opinion in Solid State and Materials Science, 2013, 17, 298-304.	5.6	31
75	An ab initio investigation of the effect of alloying elements on the elastic properties and magnetic behavior of Ni3Al. Computational Materials Science, 2015, 101, 39-46.	1.4	31
76	Thermal transport properties of MgO and Nd2Zr2O7 pyrochlore by molecular dynamics simulation. Journal of Nuclear Materials, 2008, 380, 1-7.	1.3	30
77	Atomic-Level Simulation of Ferroelectricity in Oxides: Current Status and Opportunities. Annual Review of Materials Research, 2007, 37, 239-270.	4.3	29
78	Mechanisms of Zr surface corrosion determined via molecular dynamics simulations with charge-optimized many-body (COMB) potentials. Journal of Nuclear Materials, 2014, 452, 285-295.	1.3	29
79	Interfacial phonon scattering in semiconductor nanowires by molecular-dynamics simulation. Journal of Applied Physics, 2006, 99, 123715.	1.1	28
80	The effect of normal load on polytetrafluoroethylene tribology. Journal of Physics Condensed Matter, 2009, 21, 144201.	0.7	28
81	Grain-boundary source/sink behavior for point defects: An atomistic simulation study. International Journal of Materials Research, 2009, 100, 550-555.	0.1	28
82	Data-Driven Model for Estimation of Friction Coefficient Via Informatics Methods. Tribology Letters, 2012, 47, 211-221.	1.2	28
83	Nanoindentation of Zr by molecular dynamics simulation. Journal of Nuclear Materials, 2015, 467, 742-757.	1.3	28
84	Effect of pores and He bubbles on the thermal transport properties of UO2 by molecular dynamics simulation. Journal of Nuclear Materials, 2015, 456, 253-259.	1.3	28
85	Effect of inversion on thermoelastic and thermal transport properties of MgAl2O4 spinel by atomistic simulation. Journal of Materials Science, 2011, 46, 55-62.	1.7	27
86	Atomistic simulations of the adsorption and migration barriers of Cu adatoms on ZnO surfaces using COMB potentials. Surface Science, 2012, 606, 1280-1288.	0.8	27
87	Impact of homogeneous strain on uranium vacancy diffusion in uranium dioxide. Physical Review B, 2015, 91, .	1.1	27
88	Metric for strong intrinsic fourth-order phonon anharmonicity. Physical Review B, 2017, 95, .	1.1	26
89	Effect of ionic polarizability on oxygen diffusion in Î´-Bi2O3 from atomistic simulation. Ionics, 2010, 16, 297-303.	1.2	25
90	Influence of the Molecular Level Structure of Polyethylene and Polytetrafluoroethylene on Their Tribological Response. Tribology Letters, 2011, 42, 193-201.	1.2	25

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91	Phonon-mediated thermal transport: Confronting theory and microscopic simulation with experiment. Current Opinion in Solid State and Materials Science, 2013, 17, 1-9.	5.6	25
92	Deformation processes in polycrystalline Zr by molecular dynamics simulations. Journal of Nuclear Materials, 2015, 462, 147-159.	1.3	25
93	Properties of Ti/TiC Interfaces from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 12530-12538.	1.5	25
94	Electronic structures and magnetism of Zr-, Th-, and U-based metal-organic frameworks (MOFs) by density functional theory. Computational Materials Science, 2020, 184, 109903.	1.4	25
95	Phononâ€Mediated Thermal Conductivity in Ionic Solids by Lattice Dynamicsâ€Based Methods. Journal of the American Ceramic Society, 2011, 94, 3523-3531.	1.9	24
96	Classical interatomic potential for orthorhombic uranium. Journal of Physics Condensed Matter, 2012, 24, 235403.	0.7	23
97	Charge-optimized many-body (COMB) potential for zirconium. Journal of Nuclear Materials, 2013, 441, 274-279.	1.3	23
98	Dynamical properties of AlN nanostructures and heterogeneous interfaces predicted using COMB potentials. Computational Materials Science, 2016, 113, 80-87.	1.4	23
99	Shock compression of Cu x Zr100â^'x metallic glasses from molecular dynamics simulations. Journal of Materials Science, 2018, 53, 5719-5732.	1.7	23
100	Atomistic Simulations of Integranular Fracture in Symmetric-Tilt Grain Boundaries. Journal of Materials Science, 1999, 7, 45-55.	1.2	22
101	Optimized many body potential for fcc metals. Philosophical Magazine Letters, 2009, 89, 136-144.	0.5	22
102	Kinetically driven point-defect clustering in irradiated MgO by molecular-dynamics simulation. Scripta Materialia, 2009, 60, 691-694.	2.6	21
103	A charge optimized many-body (comb) potential for titanium and titania. Journal of Physics Condensed Matter, 2014, 26, 315007.	0.7	21
104	Charge Optimized Many Body (COMB) potentials for simulation of nuclear fuel and clad. Computational Materials Science, 2018, 148, 231-241.	1.4	21
105	Generation and characterization of an improved carbon fiber model by molecular dynamics. Carbon, 2021, 173, 232-244.	5.4	21
106	Interfacial thermal conductivity: Insights from atomic level simulation. Journal of Materials Science, 2005, 40, 3143-3148.	1.7	20
107	The role of charge and ionic radius on fission product segregation to a model UO2 grain boundary. Journal of Applied Physics, 2013, 113, .	1.1	20
108	Introduction to thermal transport. Materials Today, 2005, 8, 18-20.	8.3	19

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109	Shape of ferroelectric domains in LiNbO3 and LiTaO3 from defect/domain-wall interactions. Applied Physics Letters, 2011, 98, .	1.5	19
110	The evolution of interaction between grain boundary and irradiation-induced point defects: Symmetric tilt GB in tungsten. Journal of Nuclear Materials, 2018, 500, 42-49.	1.3	19
111	Atomic-level deformation of Cu_xZr₁₀₀₋_x metallic glasses under shock loading. Journal of Applied Physics, 2018, 123, 215101.	1.1	19
112	Stabilization Mechanisms of LaFeO3 (010) Surfaces Determined with First Principles Calculations. Journal of the American Ceramic Society, 2011, 94, 1931-1939.	1.9	18
113	Structure of Î´-Bi2O3 from density functional theory: A systematic crystallographic analysis. Journal of Solid State Chemistry, 2009, 182, 1222-1228.	1.4	17
114	A charge-optimized many-body potential for the Uâ€“UO₂â€“O₂system. Journal of Physics Condensed Matter, 2013, 25, 505401.	0.7	17
115	xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">M</mml:mi><mml:msub><mml:mi mathvariant="normal">g</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>X</mml:mi></mml:mrow></mml:math><mml:mat		

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127	Thermal conductivity of argon at high pressure from first principles calculations. Journal of Applied Physics, 2013, 114, 064902.	1.1	14
128	Lattice expansion by intrinsic defects in uranium by molecular dynamics simulation. Journal of Nuclear Materials, 2016, 475, 6-18.	1.3	14
129	Heterometallic multinuclear nodes directing MOF electronic behavior. Chemical Science, 2020, 11, 7379-7389.	3.7	14
130	Effect of the initial temperature on the shock response of Cu50Zr50 bulk metallic glass by molecular dynamics simulation. Journal of Applied Physics, 2021, 129, .	1.1	14
131	High-temperature oxidation of carbon fiber and char by molecular dynamics simulation. Carbon, 2021, 185, 449-463.	5.4	14
132	Grain Boundaries in Silicon from Zero Temperature through Melting. Journal of the American Ceramic Society, 1990, 73, 933-937.	1.9	13
133	Effect of simulation conditions on friction in polytetrafluoroethylene (PTFE). Journal of Computer-Aided Materials Design, 2007, 14, 239-246.	0.7	13
134	Potential Optimization Software for Materials (POSMat). Computer Physics Communications, 2016, 203, 201-211.	3.0	13
135	Adhesion and diffusion at TiN/TiO2 interfaces: A first principles study. Computational Materials Science, 2017, 130, 249-256.	1.4	13
136	Order-disorder behavior in KNbO3 and KNbO3/KTaO3 solid solutions and superlattices by molecular-dynamics simulation. Journal of Materials Science, 2005, 40, 3213-3217.	1.7	12
137	Morphology and growth modes of metal-oxides deposited on SrTiO3. Surface Science, 2009, 603, 873-880.	0.8	12
138	Thermal conductivity of UO2 fuel: Predicting fuel performance from simulation. Jom, 2011, 63, 73-79.	0.9	12
139	Critical assessment of classical potentials for MgSiO3 perovskite with application to thermal conductivity calculations. Physics of the Earth and Planetary Interiors, 2012, 210-211, 75-89.	0.7	12
140	Overcoming the Interfacial Lattice Mismatch: Geometry Control of Goldâ€“Nickel Bimetallic Heteronanostructures. Particle and Particle Systems Characterization, 2018, 35, 1700361.	1.2	12
141	Sequestration of Radionuclides in Metalâ€“Organic Frameworks from Density Functional Theory Calculations. Journal of Physical Chemistry C, 2019, 123, 26842-26855.	1.5	12
142	A third-generation charge optimized many body (COMB3) potential for nitrogen-containing organic molecules. Computational Materials Science, 2017, 139, 153-161.	1.4	11
143	The Conundrum of Relaxation Volumes in First-Principles Calculations of Charged Defects in UO2. Applied Sciences (Switzerland), 2019, 9, 5276.	1.3	11
144	The influence of alloying on the stacking fault energy of gold from density functional theory calculations. Computational Materials Science, 2021, 188, 110236.	1.4	11

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145	Interatomic potential for the structure and energetics of tetrahedrally coordinated silica polymorphs. Physical Review B, 2007, 75, .	1.1	10
146	Surface diffusion on SrTiO3 (100): A temperature accelerated dynamics and first principles study. Surface Science, 2013, 617, 237-241.	0.8	10
147	Interaction between voids and grain boundaries in UO2 by molecular-dynamics simulation. Journal of Nuclear Materials, 2014, 448, 53-61.	1.3	10
148	Computational discovery of lanthanide doped and Co-doped Y3Al5O12 for optoelectronic applications. Applied Physics Letters, 2015, 107, 112109.	1.5	10
149	Thermodynamics and kinetics of ordered and disordered Cu/Au alloys from first principles calculations. Journal of Alloys and Compounds, 2019, 809, 151615.	2.8	10
150	Effect of Fluorocarbon Molecules Confined between Sliding Self-Mated PTFE Surfaces. Langmuir, 2011, 27, 9910-9919.	1.6	9
151	Heterometallic Actinideâ€Containing Photoresponsive Metalâ€Organic Frameworks: Dynamic and Static Tuning of Electronic Properties. Angewandte Chemie, 2021, 133, 8152-8160.	1.6	9
152	Thermal conductivity of the nâ€‰=â€‰1â€“5 and 10 members of the (SrTiO3)nSrO Ruddlesdenâ€“Popper superlattices. Applied Physics Letters, 2021, 118, .	1.5	9
153	Crossover in thermal transport mechanism in nanocrystalline silicon. Applied Physics Letters, 2006, 88, 141908.	1.5	8
154	Segregation of ruthenium to edge dislocations in uranium dioxide. Journal of Nuclear Materials, 2013, 441, 96-102.	1.3	8
155	A Mechanism for TiO₂ Formation on Stepped TiN(001) from First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 384-388.	1.5	8
156	Charge optimized many-body (COMB) potential for dynamical simulation of Niâ€“Al phases. Journal of Physics Condensed Matter, 2015, 27, 336302.	0.7	8
157	Depinning of the ferroelectric domain wall in congruent LiNbO3. Applied Physics Letters, 2016, 109, .	1.5	8
158	A Cellular Automaton Approach to the Simulation of Active Self-Assembly of Kinesin-Powered Molecular Shuttles. Journal of Computational and Theoretical Nanoscience, 2011, 8, 1999-2005.	0.4	7
159	Design of Low Wear Polymer Composites. Tribology Letters, 2012, 45, 79-87.	1.2	7
160	Charge optimized many-body potential for aluminum. Journal of Physics Condensed Matter, 2015, 27, 015003.	0.7	7
161	Elastic and thermal properties of hexagonal perovskites. Computational Materials Science, 2016, 122, 139-145.	1.4	7
162	Titanium-Carbide Formation at Defective Curved Graphene-Titanium Interfaces. MRS Advances, 2018, 3, 457-462.	0.5	7

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163	Dynamics of graphene/Al interfaces using COMB3 potentials. Physical Review Materials, 2019, 3, .	0.9	7
164	Toward an Atomistically Informed Fuel Performance Code: Thermal Properties Using FRAPCON and Molecular Dynamics Simulation. Nuclear Technology, 2009, 165, 308-312.	0.7	6
165	Lattice stability and point defect energetics of TiSi2 and TiGe2 allotropes from first-principles calculations. Journal of Applied Physics, 2021, 129, .	1.1	6
166	Study of Incorporating Cesium into Copper Hexacyanoferrate by Density Functional Theory Calculations. Journal of Physical Chemistry C, 2021, 125, 24273-24283.	1.5	6
167	Molecular dynamics simulations of SrTiO3thin-film growth from cluster deposition. Journal of Physics Condensed Matter, 2010, 22, 045001.	0.7	4
168	Role of electronic effects on the incorporation of Cr at a Î£5 grain boundary in UO2. Computational Materials Science, 2013, 78, 29-33.	1.4	4
169	Phase-field modeling of carbon fiber oxidation coupled with heat conduction. Computational Materials Science, 2022, 204, 111156.	1.4	4
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171	Publisher's Note: Second-generation charge-optimized many-body potential for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Si</mml:mtext><mml:mo>/</mml:mo><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext> amorphous silica [Phys. Rev. B82, 235302 (2010)]. Physical Review B, 2010, 82, .	1.1	3
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