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	Phase-field modeling of carbon fiber oxidation coupled with heat conduction. Computational Materials Science, 2022, 204, 111156.	1.4	4
2	Molecular dynamics simulation of the shock response of materials: A tutorial. Journal of Applied Physics, 2022, 131, .	1.1	32
3	Generation and characterization of an improved carbon fiber model by molecular dynamics. Carbon, 2021, 173, 232-244.	5.4	21
4	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
5	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
6	Heterometallic Actinideâ€Containing Photoresponsive Metalâ€Organic Frameworks: Dynamic and Static Tuning of Electronic Properties. Angewandte Chemie, 2021, 133, 8152-8160.	1.6	9
7	Lattice stability and point defect energetics of TiSi2 and TiGe2 allotropes from first-principles calculations. Journal of Applied Physics, 2021, 129, .	1.1	6
8	Frontispiece: Heterometallic Actinideâ€Containing Photoresponsive Metalâ€Organic Frameworks: Dynamic and Static Tuning of Electronic Properties. Angewandte Chemie - International Edition, 2021, 60, .	7.2	0
9	Frontispiz: Heterometallic Actinideâ€Containing Photoresponsive Metalâ€Organic Frameworks: Dynamic and Static Tuning of Electronic Properties. Angewandte Chemie, 2021, 133, .	1.6	0
10	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
11	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
12	High-temperature oxidation of carbon fiber and char by molecular dynamics simulation. Carbon, 2021, 185, 449-463.	5.4	14
13	Study of Incorporating Cesium into Copper Hexacyanoferrate by Density Functional Theory Calculations. Journal of Physical Chemistry C, 2021, 125, 24273-24283.	1.5	6
14	Nanoindentation of ZrH2 by molecular dynamics simulation. Journal of Nuclear Materials, 2020, 540, 152391.	1.3	2
15	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
16	Heterometallic multinuclear nodes directing MOF electronic behavior. Chemical Science, 2020, 11, 7379-7389.	3.7	14
17	Stability of epitaxial pseudocubic group IV-V semiconductors. Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2019, 37, 050602.	0.6	1
18	Sequestration of Radionuclides in Metalâ€“Organic Frameworks from Density Functional Theory Calculations. Journal of Physical Chemistry C, 2019, 123, 26842-26855.	1.5	12

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19	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
20	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
21	Void collapse and subsequent spallation in Cu50Zr50 metallic glass under shock loading by molecular dynamics simulations. Journal of Applied Physics, 2019, 125, .	1.1	16
22	The Conundrum of Relaxation Volumes in First-Principles Calculations of Charged Defects in UO2. Applied Sciences (Switzerland), 2019, 9, 5276.	1.3	11
23	Lattice thermal conductivity of quartz at high pressure and temperature from the Boltzmann transport equation. Journal of Applied Physics, 2019, 126, 215106.	1.1	3
24	Dynamics of graphene/Al interfaces using COMB3 potentials. Physical Review Materials, 2019, 3, .	0.9	7
25	Overcoming the Interfacial Lattice Mismatch: Geometry Control of Goldâ€“Nickel Bimetallic Heteronanostructures. Particle and Particle Systems Characterization, 2018, 35, 1700361.	1.2	12
26	Charge Optimized Many Body (COMB) potentials for simulation of nuclear fuel and clad. Computational Materials Science, 2018, 148, 231-241.	1.4	21
27	Titanium-Carbide Formation at Defective Curved Graphene-Titanium Interfaces. MRS Advances, 2018, 3, 457-462.	0.5	7
28	Effects of grain boundaries on irradiation-induced defects in tungsten by molecular dynamics simulations. Journal of Iron and Steel Research International, 2018, 25, 200-206.	1.4	2
29	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
30	Galvanic Replacement-Driven Transformations of Atomically Intermixed Bimetallic Colloidal Nanocrystals: Effects of Compositional Stoichiometry and Structural Ordering. Langmuir, 2018, 34, 4340-4350.	1.6	16
31	Shock compression of Cu x Zr100â^'x metallic glasses from molecular dynamics simulations. Journal of Materials Science, 2018, 53, 5719-5732.	1.7	23
32	Entropy contributions to phase stability in binary random solid solutions. Npj Computational Materials, 2018, 4, .	3.5	64
33	Atomic-level deformation of Cu_xZr₁₀₀₋_x metallic glasses under shock loading. Journal of Applied Physics, 2018, 123, 215101.	1.1	19
34	Hierarchical Materials as Tailored Nuclear Waste Forms: A Perspective. Chemistry of Materials, 2018, 30, 4475-4488.	3.2	98
35	Nanoindentation of ZrO2 and ZrO2/Zr systems by molecular dynamics simulation. Journal of Nuclear Materials, 2017, 486, 250-266.	1.3	17
36	Adhesion and diffusion at TiN/TiO2 interfaces: A first principles study. Computational Materials Science, 2017, 130, 249-256.	1.4	13

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37	Mechanistic materials modeling for nuclear fuel performance. Annals of Nuclear Energy, 2017, 105, 11-24.	0.9	57
38	Grapheneâ€“Titanium Interfaces from Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2017, 9, 33288-33297.	4.0	37
39	Metric for strong intrinsic fourth-order phonon anharmonicity. Physical Review B, 2017, 95, .	1.1	26
40	A third-generation charge optimized many body (COMB3) potential for nitrogen-containing organic molecules. Computational Materials Science, 2017, 139, 153-161.	1.4	11
41	Depinning of the ferroelectric domain wall in congruent LiNbO3. Applied Physics Letters, 2016, 109, .	1.5	8
42	Elastic and thermal properties of hexagonal perovskites. Computational Materials Science, 2016, 122, 139-145.	1.4	7
43	Properties of Ti/TiC Interfaces from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 12530-12538.	1.5	25
44	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
45	Effect of Surface Chemistry on Water Interaction with Cu(111). Langmuir, 2016, 32, 8061-8070.	1.6	16
46	Dynamical properties of AlN nanostructures and heterogeneous interfaces predicted using COMB potentials. Computational Materials Science, 2016, 113, 80-87.	1.4	23
47	Lattice expansion by intrinsic defects in uranium by molecular dynamics simulation. Journal of Nuclear Materials, 2016, 475, 6-18.	1.3	14
48	Potential Optimization Software for Materials (POSMat). Computer Physics Communications, 2016, 203, 201-211.	3.0	13
49	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
50	Anharmonic properties in <mml:math 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:math		

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55	Charge optimized many-body (COMB) potential for dynamical simulation of Niâ€“Al phases. Journal of Physics Condensed Matter, 2015, 27, 336302.	0.7	8
56	Charge optimized many-body (COMB) potential for Al₂O₃materials, interfaces, and nanostructures. Journal of Physics Condensed Matter, 2015, 27, 305004.	0.7	17
57	Effect of Temperature on the Friction and Wear of PTFE by Atomic-Level Simulation. Tribology Letters, 2015, 58, 1.	1.2	38
58	Impact of homogeneous strain on uranium vacancy diffusion in uranium dioxide. Physical Review B, 2015, 91, .	1.1	27
59	Deformation processes in polycrystalline Zr by molecular dynamics simulations. Journal of Nuclear Materials, 2015, 462, 147-159.	1.3	25
60	Nanoindentation of Zr by molecular dynamics simulation. Journal of Nuclear Materials, 2015, 467, 742-757.	1.3	28
61	Anisotropy in oxidation of zirconium surfaces from density functional theory calculations. Computational Materials Science, 2015, 98, 112-116.	1.4	15
62	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
63	Role of cyberinfrastructure in educating the next generation of computational materials scientists. Integrating Materials and Manufacturing Innovation, 2014, 3, 85-89.	1.2	0
64	Thermal Conductivity in Nanocrystalline Ceria Thin Films. Journal of the American Ceramic Society, 2014, 97, 562-569.	1.9	58
65	Nanoscale thermal transport. II. 2003â€“2012. Applied Physics Reviews, 2014, 1, 011305.	5.5	1,277
66	Cu cluster deposition on ZnO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si10.gif" overflow="scroll"><mml:mfenced open="(") Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 312 Td (close=")"><mml:mrow><mml:mover accent="true"><mml:mn>1</mml:mn><mml:mo stretchy="true">Â¯</mml:mo></mml:mover><mml:mn>0</mml:mn></mml:mrow></mml:mfenced></mml:math>: Morphology and growth mode predicted from molecular dynamics simulations. Surface Science, 2014,	0.8	16
67	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
68	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></mml Physical Review B, 2014, 89, .	1.1	45
69	A charge optimized many-body (comb) potential for titanium and titania. Journal of Physics Condensed Matter, 2014, 26, 315007.	0.7	21
70	Interaction between voids and grain boundaries in UO2 by molecular-dynamics simulation. Journal of Nuclear Materials, 2014, 448, 53-61.	1.3	10
71	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
72	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

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73	Uncertainty Quantification in Multiscale Simulation of Materials: A Prospective. Annual Review of Materials Research, 2013, 43, 157-182.	4.3	94
74	Surface diffusion on SrTiO3 (100): A temperature accelerated dynamics and first principles study. Surface Science, 2013, 617, 237-241.	0.8	10
75	Fitting empirical potentials: Challenges and methodologies. Current Opinion in Solid State and Materials Science, 2013, 17, 263-270.	5.6	44
76	NSF cyberinfrastructures: A new paradigm for advancing materials simulation. Current Opinion in Solid State and Materials Science, 2013, 17, 298-304.	5.6	31
77	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
78	Effects of edge dislocations on thermal transport in UO2. Journal of Nuclear Materials, 2013, 434, 203-209.	1.3	44
79	Charge-optimized many-body (COMB) potential for zirconium. Journal of Nuclear Materials, 2013, 441, 274-279.	1.3	23
80	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
81	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
82	Segregation of ruthenium to edge dislocations in uranium dioxide. Journal of Nuclear Materials, 2013, 441, 96-102.	1.3	8
83	Reactive Potentials for Advanced Atomistic Simulations. Annual Review of Materials Research, 2013, 43, 109-129.	4.3	184
84	A charge-optimized many-body potential for the Uâ€“UO₂â€“O₂system. Journal of Physics Condensed Matter, 2013, 25, 505401.	0.7	17
85	Band gap and structure of single crystal BiI3: Resolving discrepancies in literature. Journal of Applied Physics, 2013, 114, .	1.1	109
86	Thermal conductivity of argon at high pressure from first principles calculations. Journal of Applied Physics, 2013, 114, 064902.	1.1	14
87	Local probing of the interaction between intrinsic defects and ferroelectric domain walls in lithium niobate. Applied Physics Letters, 2013, 102, .	1.5	16
88	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
89	Low thermal conductivity oxides. MRS Bulletin, 2012, 37, 917-922.	1.7	298
90	Variable charge many-body interatomic potentials. MRS Bulletin, 2012, 37, 504-512.	1.7	58

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91	Variable Charge Reactive Potential for Hydrocarbons to Simulate Organic-Copper Interactions. Journal of Physical Chemistry A, 2012, 116, 7976-7991.	1.1	91
92	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
93	Critical assessment of UO2 classical potentials for thermal conductivity calculations. Journal of Materials Science, 2012, 47, 7693-7702.	1.7	48
94	Molecular dynamics investigation of the lubrication mechanism of carbon nano-onions. Computational Materials Science, 2012, 54, 91-96.	1.4	39
95	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
96	Solubility and clustering of ruthenium fission products in uranium dioxide as determined by density functional theory. Physical Review B, 2012, 85, .	1.1	15
97	Classical interatomic potential for orthorhombic uranium. Journal of Physics Condensed Matter, 2012, 24, 235403.	0.7	23
98	Data-Driven Model for Estimation of Friction Coefficient Via Informatics Methods. Tribology Letters, 2012, 47, 211-221.	1.2	28
99	Atomistic study of grain boundary sink strength under prolonged electron irradiation. Journal of Nuclear Materials, 2012, 422, 69-76.	1.3	40
100	Design of Low Wear Polymer Composites. Tribology Letters, 2012, 45, 79-87.	1.2	7
101	Effect of Fluorocarbon Molecules Confined between Sliding Self-Mated PTFE Surfaces. Langmuir, 2011, 27, 9910-9919.	1.6	9
102	Energetics of Oxidation in MoS₂Nanoparticles by Density Functional Theory. Journal of Physical Chemistry C, 2011, 115, 10606-10616.	1.5	55
103	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	1.1	47
104	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
105	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
106	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
107	Microtubule nanospool formation by active self-assembly is not initiated by thermal activation. Soft Matter, 2011, 7, 3108-3115.	1.2	33
108	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

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109	Stabilization Mechanisms of LaFeO3 (010) Surfaces Determined with First Principles Calculations. Journal of the American Ceramic Society, 2011, 94, 1931-1939.	1.9	18
110	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
111	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
112	Influence of the Molecular Level Structure of Polyethylene and Polytetrafluoroethylene on Their Tribological Response. Tribology Letters, 2011, 42, 193-201.	1.2	25
113	Thermal conductivity of UO2 fuel: Predicting fuel performance from simulation. Jom, 2011, 63, 73-79.	0.9	12
114	Modeling reaction pathways of low energy particle deposition on thiophene via ab initio calculations. Chemical Physics Letters, 2011, 510, 197-201.	1.2	2
115	Structure and energetics of 180Â° domain walls in PbTiO₃by density functional theory. Journal of Physics Condensed Matter, 2011, 23, 175902.	0.7	48
116	Shape of ferroelectric domains in LiNbO3 and LiTaO3 from defect/domain-wall interactions. Applied Physics Letters, 2011, 98, .	1.5	19
117	Interactions of Defects and Domain Walls in LiNbO₃â€“ Insights from Simulations. IOP Conference Series: Materials Science and Engineering, 2010, 15, 012003.	0.3	3
118	Effect of ionic polarizability on oxygen diffusion in Î´-Bi2O3 from atomistic simulation. Ionics, 2010, 16, 297-303.	1.2	25
119	Anisotropic thermal properties in orthorhombic perovskites. Journal of Materials Science, 2010, 45, 168-176.	1.7	14
120	A critical assessment of interatomic potentials for ceria with application to its elastic properties. Solid State Ionics, 2010, 181, 551-556.	1.3	42
121	Preface to Special Topic: Selected Papers from the Fourth International Conference on Multiscale Materials Modeling, Tallahassee, Florida, USA, 2008. Journal of Applied Physics, 2010, 107, 061701.	1.1	0
122	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:r atomic-level simulations. Physical Review B, 2010, 82, .	1.1	45
123	ZhaoetÂal.Reply:. Physical Review Letters, 2010, 105, .	2.9	2
124	Molecular dynamics simulations of SrTiO3thin-film growth from cluster deposition. Journal of Physics Condensed Matter, 2010, 22, 045001.	0.7	4
125	Molecular dynamics simulation of metal oxide growth on SiTiO 3. Proceedings of SPIE, 2010, , .	0.8	0
126	Evaluation of computational techniques for solving the Boltzmann transport equation for lattice thermal conductivity calculations. Physical Review B, 2010, 82, .	1.1	69

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127	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></mml:mrow></mml:msub></mml:mrow></mml:math> amorphous silica [Phys. Rev. B82, 235302 (2010)]. Physical Review B, 2010, 82, .	1.1	3
128	Charge-optimized many-body potential for the hafnium/hafnium oxide system. Physical Review B, 2010, 81, .	1.1	130
129	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></mml:mrow></mml:msub></mml:mrow></mml:math> amorphous silica. Physical Review B, 2010, 82, .	1.1	80
130	Structure and diffusion of intrinsic defect complexes in LiNbO₃from density functional theory calculations. Journal of Physics Condensed Matter, 2010, 22, 135002.	0.7	39
131	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:msub></mml:mrow></mml:math> Physical Review B, 2010, 82, .	1.1	41
132	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:msub></mml:mrow></mml:math> first-principles and thermodynamic calculations. Physical Review B, 2009, 80, .	1.1	35
133	Transition from Thermal to Athermal Friction under Cryogenic Conditions. Physical Review Letters, 2009, 102, 186102.	2.9	73
134	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:msub></mml:mrow></mml:math> molecular dynamics simulation. Physical Review B, 2009, 80, .	1.1	40
135	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
136	Crossover in thermal transport properties of natural, perovskite-structured superlattices. Applied Physics Letters, 2009, 95, .	1.5	42
137	A computational study of SrTiO₃ thin film deposition: Morphology and growth modes. Journal of Materials Research, 2009, 24, 1994-2000.	1.2	2
138	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
139	The effect of normal load on polytetrafluoroethylene tribology. Journal of Physics Condensed Matter, 2009, 21, 144201.	0.7	28
140	Kinetically driven point-defect clustering in irradiated MgO by molecular-dynamics simulation. Scripta Materialia, 2009, 60, 691-694.	2.6	21
141	Morphology and growth modes of metal-oxides deposited on SrTiO3. Surface Science, 2009, 603, 873-880.	0.8	12
142	Thermal Transport in Offâ€Stoichiometric Uranium Dioxide by Atomic Level Simulation. Journal of the American Ceramic Society, 2009, 92, 850-856.	1.9	47
143	Energetics of intrinsic point defects in uranium dioxide from electronic-structure calculations. Journal of Nuclear Materials, 2009, 384, 61-69.	1.3	127
144	Structure of Î´-Bi2O3 from density functional theory: A systematic crystallographic analysis. Journal of Solid State Chemistry, 2009, 182, 1222-1228.	1.4	17

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145	Optimized many body potential for fcc metals. Philosophical Magazine Letters, 2009, 89, 136-144.	0.5	22
146	Parametrization of a reactive many-body potential for Moâ€“S systems. Physical Review B, 2009, 79, .	1.1	241
147	Simulating Multifunctional Structures. Science, 2009, 325, 1634-1635.	6.0	34
148	Grain-boundary source/sink behavior for point defects: An atomistic simulation study. International Journal of Materials Research, 2009, 100, 550-555.	0.1	28
149	Toward an Atomistically Informed Fuel Performance Code: Thermal Properties Using FRAPCON and Molecular Dynamics Simulation. Nuclear Technology, 2009, 165, 308-312.	0.7	6
150	Thermal transport properties of MgO and Nd2Zr2O7 pyrochlore by molecular dynamics simulation. Journal of Nuclear Materials, 2008, 380, 1-7.	1.3	30
151	Thermal transport properties of uranium dioxide by molecular dynamics simulations. Journal of Nuclear Materials, 2008, 375, 388-396.	1.3	87
152	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
153	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	1.1	109
154	First-principles determination of static 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
155	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
156	Thermal conductance across grain boundaries in diamond from molecular dynamics simulation. Journal of Applied Physics, 2007, 102, 063503.	1.1	47
157	Sliding orientation effects on the tribological properties of polytetrafluoroethylene. Journal of Applied Physics, 2007, 102, .	1.1	54
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