

# Simon R Phillpot

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

179  
papers

11,543  
citations

43  
h-index

104  
g-index

188  
ext. papers

12,785  
ext. citations

4.8  
avg, IF

6.21  
L-index

#	Paper	IF	Citations
179	Molecular dynamics simulation of the shock response of materials: A tutorial. <i>Journal of Applied Physics</i> , <b>2022</b> , 131, 051101	2.5	3
178	Phase-field modeling of carbon fiber oxidation coupled with heat conduction. <i>Computational Materials Science</i> , <b>2022</b> , 204, 111156	3.2	1
177	Thermal conductivity of the n = 18 and 10 members of the (SrTiO <sub>3</sub> ) <sub>n</sub> SrO Ruddlesden-Popper superlattices. <i>Applied Physics Letters</i> , <b>2021</b> , 118, 091904	3.4	4
176	Effect of the initial temperature on the shock response of Cu <sub>50</sub> Zr <sub>50</sub> bulk metallic glass by molecular dynamics simulation. <i>Journal of Applied Physics</i> , <b>2021</b> , 129, 165103	2.5	5
175	Generation and characterization of an improved carbon fiber model by molecular dynamics. <i>Carbon</i> , <b>2021</b> , 173, 232-244	10.4	7
174	The influence of alloying on the stacking fault energy of gold from density functional theory calculations. <i>Computational Materials Science</i> , <b>2021</b> , 188, 110236	3.2	3
173	Heterometallic Actinide-Containing Photoresponsive Metal-Organic Frameworks: Dynamic and Static Tuning of Electronic Properties. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 8072-8080	16.4	13
172	Heterometallic Actinide-Containing Photoresponsive Metal-Organic Frameworks: Dynamic and Static Tuning of Electronic Properties. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 8152-8160	3.6	3
171	Lattice stability and point defect energetics of TiSi <sub>2</sub> and TiGe <sub>2</sub> allotropes from first-principles calculations. <i>Journal of Applied Physics</i> , <b>2021</b> , 129, 085104	2.5	1
170	High-temperature oxidation of carbon fiber and char by molecular dynamics simulation. <i>Carbon</i> , <b>2021</b> , 185, 449-463	10.4	3
169	Electronic structures and magnetism of Zr-, Th-, and U-based metal-organic frameworks (MOFs) by density functional theory. <i>Computational Materials Science</i> , <b>2020</b> , 184, 109903	3.2	7
168	Heterometallic multinuclear nodes directing MOF electronic behavior. <i>Chemical Science</i> , <b>2020</b> , 11, 7379-7389	13.9	5
167	Nanoindentation of ZrH <sub>2</sub> by molecular dynamics simulation. <i>Journal of Nuclear Materials</i> , <b>2020</b> , 540, 152391	3.9	1
166	Thermodynamics and kinetics of ordered and disordered Cu/Au alloys from first principles calculations. <i>Journal of Alloys and Compounds</i> , <b>2019</b> , 809, 151615	5.7	2
165	Thermodynamics and Electronic Properties of Heterometallic Multinuclear Actinide-Containing Metal-Organic Frameworks with "Structural Memory". <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 11628-11640	16.4	42
164	Void collapse and subsequent spallation in Cu <sub>50</sub> Zr <sub>50</sub> metallic glass under shock loading by molecular dynamics simulations. <i>Journal of Applied Physics</i> , <b>2019</b> , 125, 215903	2.5	7
163	Stability of epitaxial pseudocubic group IV-V semiconductors. <i>Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics</i> , <b>2019</b> , 37, 050602	1.3	

162	Sequestration of Radionuclides in Metal-Organic Frameworks from Density Functional Theory Calculations. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 26842-26855	3.8	5
161	Dynamics of graphene/Al interfaces using COMB3 potentials. <i>Physical Review Materials</i> , <b>2019</b> , 3,	3.2	2
160	The Conundrum of Relaxation Volumes in First-Principles Calculations of Charged Defects in UO <sub>2</sub> . <i>Applied Sciences (Switzerland)</i> , <b>2019</b> , 9, 5276	2.6	7
159	Lattice thermal conductivity of quartz at high pressure and temperature from the Boltzmann transport equation. <i>Journal of Applied Physics</i> , <b>2019</b> , 126, 215106	2.5	0
158	Overcoming the Interfacial Lattice Mismatch: Geometry Control of Gold-Nickel Bimetallic Heteronanostructures. <i>Particle and Particle Systems Characterization</i> , <b>2018</b> , 35, 1700361	3.1	4
157	Charge Optimized Many Body (COMB) potentials for simulation of nuclear fuel and clad. <i>Computational Materials Science</i> , <b>2018</b> , 148, 231-241	3.2	14
156	Titanium-Carbide Formation at Defective Curved Graphene-Titanium Interfaces. <i>MRS Advances</i> , <b>2018</b> , 3, 457-462	0.7	4
155	Effects of grain boundaries on irradiation-induced defects in tungsten by molecular dynamics simulations. <i>Journal of Iron and Steel Research International</i> , <b>2018</b> , 25, 200-206	1.2	2
154	The evolution of interaction between grain boundary and irradiation-induced point defects: Symmetric tilt GB in tungsten. <i>Journal of Nuclear Materials</i> , <b>2018</b> , 500, 42-49	3.3	13
153	Galvanic Replacement-Driven Transformations of Atomically Intermixed Bimetallic Colloidal Nanocrystals: Effects of Compositional Stoichiometry and Structural Ordering. <i>Langmuir</i> , <b>2018</b> , 34, 4340-4350	4.350	10
152	Shock compression of Cu x Zr <sub>100-x</sub> metallic glasses from molecular dynamics simulations. <i>Journal of Materials Science</i> , <b>2018</b> , 53, 5719-5732	4.3	13
151	Hierarchical Materials as Tailored Nuclear Waste Forms: A Perspective. <i>Chemistry of Materials</i> , <b>2018</b> , 30, 4475-4488	9.6	69
150	Entropy contributions to phase stability in binary random solid solutions. <i>Npj Computational Materials</i> , <b>2018</b> , 4,	10.9	33
149	Atomic-level deformation of Cu <sub>x</sub> Zr <sub>100-x</sub> metallic glasses under shock loading. <i>Journal of Applied Physics</i> , <b>2018</b> , 123, 215101	2.5	14
148	Nanoindentation of ZrO <sub>2</sub> and ZrO <sub>2</sub> /Zr systems by molecular dynamics simulation. <i>Journal of Nuclear Materials</i> , <b>2017</b> , 486, 250-266	3.3	15
147	Adhesion and diffusion at TiN/TiO <sub>2</sub> interfaces: A first principles study. <i>Computational Materials Science</i> , <b>2017</b> , 130, 249-256	3.2	11
146	Mechanistic materials modeling for nuclear fuel performance. <i>Annals of Nuclear Energy</i> , <b>2017</b> , 105, 11-24	4.7	41
145	Graphene-Titanium Interfaces from Molecular Dynamics Simulations. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2017</b> , 9, 33288-33297	9.5	27

144	Metric for strong intrinsic fourth-order phonon anharmonicity. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	19
143	A third-generation charge optimized many body (COMB3) potential for nitrogen-containing organic molecules. <i>Computational Materials Science</i> , <b>2017</b> , 139, 153-161	3.2	7
142	Dynamical properties of AlN nanostructures and heterogeneous interfaces predicted using COMB potentials. <i>Computational Materials Science</i> , <b>2016</b> , 113, 80-87	3.2	13
141	Lattice expansion by intrinsic defects in uranium by molecular dynamics simulation. <i>Journal of Nuclear Materials</i> , <b>2016</b> , 475, 6-18	3.3	8
140	Potential Optimization Software for Materials (POSMat). <i>Computer Physics Communications</i> , <b>2016</b> , 203, 201-211	4.2	11
139	Nanoindentation of gold and gold alloys by molecular dynamics simulation. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , <b>2016</b> , 651, 346-357	5.3	39
138	Depinning of the ferroelectric domain wall in congruent LiNbO <sub>3</sub> . <i>Applied Physics Letters</i> , <b>2016</b> , 109, 082905	3.4	6
137	Elastic and thermal properties of hexagonal perovskites. <i>Computational Materials Science</i> , <b>2016</b> , 122, 139-145	3.2	7
136	Properties of Ti/TiC Interfaces from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 12530-12538	3.8	21
135	Homogeneous hydride formation path in H <sub>2</sub> Zr: Molecular dynamics simulations with the charge-optimized many-body potential. <i>Acta Materialia</i> , <b>2016</b> , 111, 357-365	8.4	27
134	Effect of Surface Chemistry on Water Interaction with Cu(111). <i>Langmuir</i> , <b>2016</b> , 32, 8061-70	4	13
133	Charge optimized many-body (COMB) potential for dynamical simulation of Ni-Al phases. <i>Journal of Physics Condensed Matter</i> , <b>2015</b> , 27, 336302	1.8	4
132	Charge optimized many-body (COMB) potential for Al <sub>2</sub> O <sub>3</sub> materials, interfaces, and nanostructures. <i>Journal of Physics Condensed Matter</i> , <b>2015</b> , 27, 305004	1.8	7
131	Effect of Temperature on the Friction and Wear of PTFE by Atomic-Level Simulation. <i>Tribology Letters</i> , <b>2015</b> , 58, 1	2.8	23
130	Impact of homogeneous strain on uranium vacancy diffusion in uranium dioxide. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	23
129	Deformation processes in polycrystalline Zr by molecular dynamics simulations. <i>Journal of Nuclear Materials</i> , <b>2015</b> , 462, 147-159	3.3	21
128	Nanoindentation of Zr by molecular dynamics simulation. <i>Journal of Nuclear Materials</i> , <b>2015</b> , 467, 742-757	3.3	22
127	Anisotropy in oxidation of zirconium surfaces from density functional theory calculations. <i>Computational Materials Science</i> , <b>2015</b> , 98, 112-116	3.2	13

126	Effect of pores and He bubbles on the thermal transport properties of UO <sub>2</sub> by molecular dynamics simulation. <i>Journal of Nuclear Materials</i> , <b>2015</b> , 456, 253-259	3.3	23
125	Anharmonic properties in Mg <sub>2</sub> X (X=C,Si,Ge,Sn,Pb) from first-principles calculations. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	10
124	Computational discovery of lanthanide doped and Co-doped Y <sub>3</sub> Al <sub>5</sub> O <sub>12</sub> for optoelectronic applications. <i>Applied Physics Letters</i> , <b>2015</b> , 107, 112109	3.4	9
123	Phonon Transport Simulator (PhonTS). <i>Computer Physics Communications</i> , <b>2015</b> , 192, 196-204	4.2	51
122	Charge optimized many-body potential for aluminum. <i>Journal of Physics Condensed Matter</i> , <b>2015</b> , 27, 015003	1.8	5
121	An ab initio investigation of the effect of alloying elements on the elastic properties and magnetic behavior of Ni <sub>3</sub> Al. <i>Computational Materials Science</i> , <b>2015</b> , 101, 39-46	3.2	22
120	Thermal Conductivity in Nanocrystalline Ceria Thin Films. <i>Journal of the American Ceramic Society</i> , <b>2014</b> , 97, 562-569	3.8	50
119	Nanoscale thermal transport. II. 2003-2012. <i>Applied Physics Reviews</i> , <b>2014</b> , 1, 011305	17.3	1050
118	Cu cluster deposition on ZnO(101̄0): Morphology and growth mode predicted from molecular dynamics simulations. <i>Surface Science</i> , <b>2014</b> , 621, 109-116	1.8	16
117	A Mechanism for TiO <sub>2</sub> Formation on Stepped TiN(001) from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 384-388	3.8	7
116	Phonon density of states and anharmonicity of UO <sub>2</sub> . <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	37
115	A charge optimized many-body (COMB) potential for titanium and titania. <i>Journal of Physics Condensed Matter</i> , <b>2014</b> , 26, 315007	1.8	20
114	Interaction between voids and grain boundaries in UO <sub>2</sub> by molecular-dynamics simulation. <i>Journal of Nuclear Materials</i> , <b>2014</b> , 448, 53-61	3.3	7
113	Mechanisms of Zr surface corrosion determined via molecular dynamics simulations with charge-optimized many-body (COMB) potentials. <i>Journal of Nuclear Materials</i> , <b>2014</b> , 452, 285-295	3.3	22
112	Role of cyberinfrastructure in educating the next generation of computational materials scientists. <i>Integrating Materials and Manufacturing Innovation</i> , <b>2014</b> , 3, 85-89	2.9	
111	Classical atomistic simulations of surfaces and heterogeneous interfaces with the charge-optimized many body (COMB) potentials. <i>Materials Science and Engineering Reports</i> , <b>2013</b> , 74, 255-279	30.9	167
110	Uncertainty Quantification in Multiscale Simulation of Materials: A Prospective. <i>Annual Review of Materials Research</i> , <b>2013</b> , 43, 157-182	12.8	74
109	Surface diffusion on SrTiO <sub>3</sub> (100): A temperature accelerated dynamics and first principles study. <i>Surface Science</i> , <b>2013</b> , 617, 237-241	1.8	9

108	Fitting empirical potentials: Challenges and methodologies. <i>Current Opinion in Solid State and Materials Science</i> , <b>2013</b> , 17, 263-270	12	39
107	NSF cyberinfrastructures: A new paradigm for advancing materials simulation. <i>Current Opinion in Solid State and Materials Science</i> , <b>2013</b> , 17, 298-304	12	25
106	Phonon-mediated thermal transport: Confronting theory and microscopic simulation with experiment. <i>Current Opinion in Solid State and Materials Science</i> , <b>2013</b> , 17, 1-9	12	22
105	Effects of edge dislocations on thermal transport in UO <sub>2</sub> . <i>Journal of Nuclear Materials</i> , <b>2013</b> , 434, 203-209	3.3	38
104	Charge-optimized many-body (COMB) potential for zirconium. <i>Journal of Nuclear Materials</i> , <b>2013</b> , 441, 274-279	3.3	20
103	Role of electronic effects on the incorporation of Cr at a $\Sigma$ grain boundary in UO <sub>2</sub> . <i>Computational Materials Science</i> , <b>2013</b> , 78, 29-33	3.2	2
102	Phonon lifetime investigation of anharmonicity and thermal conductivity of UO <sub>2</sub> by neutron scattering and theory. <i>Physical Review Letters</i> , <b>2013</b> , 110, 157401	7.4	110
101	Segregation of ruthenium to edge dislocations in uranium dioxide. <i>Journal of Nuclear Materials</i> , <b>2013</b> , 441, 96-102	3.3	8
100	Reactive Potentials for Advanced Atomistic Simulations. <i>Annual Review of Materials Research</i> , <b>2013</b> , 43, 109-129	12.8	147
99	A charge-optimized many-body potential for the U-UO <sub>2</sub> -O <sub>2</sub> system. <i>Journal of Physics Condensed Matter</i> , <b>2013</b> , 25, 505401	1.8	15
98	Band gap and structure of single crystal BiI <sub>3</sub> : Resolving discrepancies in literature. <i>Journal of Applied Physics</i> , <b>2013</b> , 114, 033110	2.5	86
97	Thermal conductivity of argon at high pressure from first principles calculations. <i>Journal of Applied Physics</i> , <b>2013</b> , 114, 064902	2.5	12
96	Local probing of the interaction between intrinsic defects and ferroelectric domain walls in lithium niobate. <i>Applied Physics Letters</i> , <b>2013</b> , 102, 042905	3.4	16
95	The role of charge and ionic radius on fission product segregation to a model UO <sub>2</sub> grain boundary. <i>Journal of Applied Physics</i> , <b>2013</b> , 113, 134902	2.5	19
94	Atomistic study of grain boundary sink strength under prolonged electron irradiation. <i>Journal of Nuclear Materials</i> , <b>2012</b> , 422, 69-76	3.3	36
93	Design of Low Wear Polymer Composites. <i>Tribology Letters</i> , <b>2012</b> , 45, 79-87	2.8	7
92	Low thermal conductivity oxides. <i>MRS Bulletin</i> , <b>2012</b> , 37, 917-922	3.2	222
91	Variable charge many-body interatomic potentials. <i>MRS Bulletin</i> , <b>2012</b> , 37, 504-512	3.2	48

90	Variable charge reactive potential for hydrocarbons to simulate organic-copper interactions. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 7976-91	2.8	76
89	Atomistic simulations of the adsorption and migration barriers of Cu adatoms on ZnO surfaces using COMB potentials. <i>Surface Science</i> , <b>2012</b> , 606, 1280-1288	1.8	26
88	Critical assessment of UO <sub>2</sub> classical potentials for thermal conductivity calculations. <i>Journal of Materials Science</i> , <b>2012</b> , 47, 7693-7702	4.3	46
87	Molecular dynamics investigation of the lubrication mechanism of carbon nano-onions. <i>Computational Materials Science</i> , <b>2012</b> , 54, 91-96	3.2	33
86	Critical assessment of classical potentials for MgSiO <sub>3</sub> perovskite with application to thermal conductivity calculations. <i>Physics of the Earth and Planetary Interiors</i> , <b>2012</b> , 210-211, 75-89	2.3	12
85	Solubility and clustering of ruthenium fission products in uranium dioxide as determined by density functional theory. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	13
84	Classical interatomic potential for orthorhombic uranium. <i>Journal of Physics Condensed Matter</i> , <b>2012</b> , 24, 235403	1.8	14
83	Data-Driven Model for Estimation of Friction Coefficient Via Informatics Methods. <i>Tribology Letters</i> , <b>2012</b> , 47, 211-221	2.8	23
82	Molecular dynamics study of the adhesion of Cu/SiO <sub>2</sub> interfaces using a variable-charge interatomic potential. <i>Physical Review B</i> , <b>2011</b> , 83,	3.3	42
81	Stoichiometry of the LaFeO <sub>3</sub> (010) surface determined from first-principles and thermodynamic calculations. <i>Physical Review B</i> , <b>2011</b> , 83,	3.3	29
80	Atomistic simulations of copper oxidation and Cu/Cu <sub>2</sub> O interfaces using charge-optimized many-body potentials. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	59
79	A Cellular Automaton Approach to the Simulation of Active Self-Assembly of Kinesin-Powered Molecular Shuttles. <i>Journal of Computational and Theoretical Nanoscience</i> , <b>2011</b> , 8, 1999-2005	0.3	7
78	Microtubule nanospool formation by active self-assembly is not initiated by thermal activation. <i>Soft Matter</i> , <b>2011</b> , 7, 3108-3115	3.6	30
77	Grain Boundaries in Uranium Dioxide: Scanning Electron Microscopy Experiments and Atomistic Simulations. <i>Journal of the American Ceramic Society</i> , <b>2011</b> , 94, 1893-1900	3.8	66
76	Stabilization Mechanisms of LaFeO <sub>3</sub> (010) Surfaces Determined with First Principles Calculations. <i>Journal of the American Ceramic Society</i> , <b>2011</b> , 94, 1931-1939	3.8	13
75	Phonon-Mediated Thermal Conductivity in Ionic Solids by Lattice Dynamics-Based Methods. <i>Journal of the American Ceramic Society</i> , <b>2011</b> , 94, 3523-3531	3.8	22
74	Effect of inversion on thermoelastic and thermal transport properties of MgAl <sub>2</sub> O <sub>4</sub> spinel by atomistic simulation. <i>Journal of Materials Science</i> , <b>2011</b> , 46, 55-62	4.3	21
73	Influence of the Molecular Level Structure of Polyethylene and Polytetrafluoroethylene on Their Tribological Response. <i>Tribology Letters</i> , <b>2011</b> , 42, 193-201	2.8	20

72	Thermal conductivity of UO <sub>2</sub> fuel: Predicting fuel performance from simulation. <i>Jom</i> , <b>2011</b> , 63, 73-79	2.1	12
71	Effect of fluorocarbon molecules confined between sliding self-mated PTFE surfaces. <i>Langmuir</i> , <b>2011</b> , 27, 9910-9	4	7
70	Energetics of Oxidation in MoS <sub>2</sub> Nanoparticles by Density Functional Theory. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 10606-10616	3.8	42
69	Modeling reaction pathways of low energy particle deposition on thiophene via ab initio calculations. <i>Chemical Physics Letters</i> , <b>2011</b> , 510, 197-201	2.5	2
68	Structure and energetics of 180° domain walls in PbTiO <sub>3</sub> by density functional theory. <i>Journal of Physics Condensed Matter</i> , <b>2011</b> , 23, 175902	1.8	37
67	Shape of ferroelectric domains in LiNbO <sub>3</sub> and LiTaO <sub>3</sub> from defect/domain-wall interactions. <i>Applied Physics Letters</i> , <b>2011</b> , 98, 092903	3.4	18
66	Preface to Special Topic: Selected Papers from the Fourth International Conference on Multiscale Materials Modeling, Tallahassee, Florida, USA, 2008. <i>Journal of Applied Physics</i> , <b>2010</b> , 107, 061701	2.5	
65	Structure and energetics of ferroelectric domain walls in LiNbO <sub>3</sub> from atomic-level simulations. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	42
64	Zhao et al. Reply:. <i>Physical Review Letters</i> , <b>2010</b> , 105,	7.4	1
63	Molecular dynamics simulations of SrTiO <sub>3</sub> thin-film growth from cluster deposition. <i>Journal of Physics Condensed Matter</i> , <b>2010</b> , 22, 045001	1.8	4
62	Evaluation of computational techniques for solving the Boltzmann transport equation for lattice thermal conductivity calculations. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	53
61	Publisher's Note: Second-generation charge-optimized many-body potential for Si/SiO <sub>2</sub> and amorphous silica [Phys. Rev. B 82, 235302 (2010)]. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	3
60	Charge-optimized many-body potential for the hafnium/hafnium oxide system. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	109
59	Second-generation charge-optimized many-body potential for Si/SiO <sub>2</sub> and amorphous silica. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	79
58	Structure and diffusion of intrinsic defect complexes in LiNbO <sub>3</sub> from density functional theory calculations. <i>Journal of Physics Condensed Matter</i> , <b>2010</b> , 22, 135002	1.8	30
57	Stability and charge transfer levels of extrinsic defects in LiNbO <sub>3</sub> . <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	38
56	Interactions of Defects and Domain Walls in LiNbO <sub>3</sub> —Insights from Simulations. <i>IOP Conference Series: Materials Science and Engineering</i> , <b>2010</b> , 15, 012003	0.4	2
55	Effect of ionic polarizability on oxygen diffusion in Bi <sub>2</sub> O <sub>3</sub> from atomistic simulation. <i>Ionics</i> , <b>2010</b> , 16, 297-303	2.7	19



54	Anisotropic thermal properties in orthorhombic perovskites. <i>Journal of Materials Science</i> , <b>2010</b> , 45, 168-176	14
53	A critical assessment of interatomic potentials for ceria with application to its elastic properties. <i>Solid State Ionics</i> , <b>2010</b> , 181, 551-556	3-3 39
52	Structure and energetics of Er defects in LiNbO3 from first-principles and thermodynamic calculations. <i>Physical Review B</i> , <b>2009</b> , 80,	3-3 33
51	Transition from thermal to athermal friction under cryogenic conditions. <i>Physical Review Letters</i> , <b>2009</b> , 102, 186102	7-4 58
50	Kinetically evolving irradiation-induced point defect clusters in UO2 by molecular dynamics simulation. <i>Physical Review B</i> , <b>2009</b> , 80,	3-3 35
49	Mixed Bloch-Néel-Ising character of 180° ferroelectric domain walls. <i>Physical Review B</i> , <b>2009</b> , 80,	3-3 121
48	Crossover in thermal transport properties of natural, perovskite-structured superlattices. <i>Applied Physics Letters</i> , <b>2009</b> , 95, 161906	3-4 41
47	A computational study of SrTiO3 thin film deposition: Morphology and growth modes. <i>Journal of Materials Research</i> , <b>2009</b> , 24, 1994-2000	2-5 2
46	Thermal transport in polyethylene and at polyethylene-diamond interfaces investigated using molecular dynamics simulation. <i>Journal of Physics Condensed Matter</i> , <b>2009</b> , 21, 084219	1-8 31
45	The effect of normal load on polytetrafluoroethylene tribology. <i>Journal of Physics Condensed Matter</i> , <b>2009</b> , 21, 144201	1-8 25
44	Kinetically driven point-defect clustering in irradiated MgO by molecular-dynamics simulation. <i>Scripta Materialia</i> , <b>2009</b> , 60, 691-694	5-6 16
43	Morphology and growth modes of metal-oxides deposited on SrTiO3. <i>Surface Science</i> , <b>2009</b> , 603, 873-880	8 11
42	Thermal Transport in Off-Stoichiometric Uranium Dioxide by Atomic Level Simulation. <i>Journal of the American Ceramic Society</i> , <b>2009</b> , 92, 850-856	3-8 47
41	Energetics of intrinsic point defects in uranium dioxide from electronic-structure calculations. <i>Journal of Nuclear Materials</i> , <b>2009</b> , 384, 61-69	3-3 118
40	Structure of Bi2O3 from density functional theory: A systematic crystallographic analysis. <i>Journal of Solid State Chemistry</i> , <b>2009</b> , 182, 1222-1228	3-3 14
39	Optimized many body potential for fcc metals. <i>Philosophical Magazine Letters</i> , <b>2009</b> , 89, 136-144	1 22
38	Parametrization of a reactive many-body potential for MoS2 systems. <i>Physical Review B</i> , <b>2009</b> , 79,	3-3 198
37	Materials science. Simulating multifunctional structures. <i>Science</i> , <b>2009</b> , 325, 1634-5	33-3 32

36	Grain-boundary source/sink behavior for point defects: An atomistic simulation study. <i>International Journal of Materials Research</i> , <b>2009</b> , 100, 550-555	0.5	25
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