# Simon R Phillpot

## List of Publications by Citations



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|---|---|---|---|
| 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 | Nanoscale thermal transport. *Journal of Applied Physics*, **2003**, 93, 793-818 | 2.5 | 2204 |
| 178 | Comparison of atomic-level simulation methods for computing thermal conductivity. *Physical Review B*, **2002**, 65, | 3.3 | 1117 |
| 177 | Nanoscale thermal transport. II. 2003–2012. *Applied Physics Reviews*, **2014**, 1, 011305 | 17.3 | 1050 |
| 176 | Dislocation processes in the deformation of nanocrystalline aluminium by molecular-dynamics simulation. *Nature Materials*, **2002**, 1, 45-8 | 27 | 762 |
| 175 | Thermal barrier coating materials. *Materials Today*, **2005**, 8, 22-29 | 21.8 | 664 |
| 174 | Low thermal conductivity oxides. *MRS Bulletin*, **2012**, 37, 917-922 | 3.2 | 222 |
| 173 | Parametrization of a reactive many-body potential for Mo–S systems. *Physical Review B*, **2009**, 79, | 3.3 | 198 |
| 172 | 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 | 30.9 | 167 |
| 171 | Scaling behavior of grain-rotation-induced grain growth. *Physical Review Letters*, **2002**, 89, 206101 | 7.4 | 161 |
| 170 | Reactive Potentials for Advanced Atomistic Simulations. *Annual Review of Materials Research*, **2013**, 43, 109-129 | 12.8 | 147 |
| 169 | Charge optimized many-body potential for the Si–SiO2 system. *Physical Review B*, **2007**, 75, | 3.3 | 132 |
| 168 | Thermal transport and grain boundary conductance in ultrananocrystalline diamond thin films. *Journal of Applied Physics*, **2006**, 99, 114301 | 2.5 | 122 |
| 167 | Mixed Bloch-Néel-Ising character of 180° ferroelectric domain walls. *Physical Review B*, **2009**, 80, | 3.3 | 121 |
| 166 | Mechanism of the Cubic-to-Tetragonal Phase Transition in Zirconia and Yttria-Stabilized Zirconia by Molecular-Dynamics Simulation. *Journal of the American Ceramic Society*, **2004**, 84, 1609-1619 | 3.8 | 119 |
| 165 | Energetics of intrinsic point defects in uranium dioxide from electronic-structure calculations. *Journal of Nuclear Materials*, **2009**, 384, 61-69 | 3.3 | 118 |
| 164 | Phonon lifetime investigation of anharmonicity and thermal conductivity of UO2 by neutron scattering and theory. *Physical Review Letters*, **2013**, 110, 157401 | 7.4 | 110 |
| 163 | Charge-optimized many-body potential for the hafnium/hafnium oxide system. *Physical Review B*, **2010**, 81, | 3.3 | 109 |

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|---|---|---|---|
| 162 | Mechanism of Thermal Transport in Zirconia and Yttria-Stabilized Zirconia by Molecular-Dynamics Simulation. *Journal of the American Ceramic Society*, **2001**, 84, 2997-3007 | 3.8 | 108 |
| 161 | Vibrations and thermal transport in nanocrystalline silicon. *Physical Review B*, **2006**, 74, | 3.3 | 97 |
| 160 | Stability of intrinsic defects and defect clusters in LiNbO3 from density functional theory calculations. *Physical Review B*, **2008**, 78, | 3.3 | 96 |
| 159 | Atomic-Scale Mechanism of Crack-Tip Plasticity: Dislocation Nucleation and Crack-Tip Shielding. *Physical Review Letters*, **1997**, 79, 1309-1312 | 7.4 | 94 |
| 158 | Atomic-level simulation of ferroelectricity in oxide materials. *Current Opinion in Solid State and Materials Science*, **2005**, 9, 107-113 | 12 | 92 |
| 157 | First-principles determination of static potential energy surfaces for atomic friction in MoS2 and MoO3. *Physical Review B*, **2008**, 77, | 3.3 | 89 |
| 156 | Band gap and structure of single crystal BiI3: Resolving discrepancies in literature. *Journal of Applied Physics*, **2013**, 114, 033110 | 2.5 | 86 |
| 155 | Thermal transport properties of uranium dioxide by molecular dynamics simulations. *Journal of Nuclear Materials*, **2008**, 375, 388-396 | 3.3 | 81 |
| 154 | Second-generation charge-optimized many-body potential for Si/SiO2 and amorphous silica. *Physical Review B*, **2010**, 82, | 3.3 | 79 |
| 153 | Variable charge reactive potential for hydrocarbons to simulate organic-copper interactions. *Journal of Physical Chemistry A*, **2012**, 116, 7976-91 | 2.8 | 76 |
| 152 | Uncertainty Quantification in Multiscale Simulation of Materials: A Prospective. *Annual Review of Materials Research*, **2013**, 43, 157-182 | 12.8 | 74 |
| 151 | Hierarchical Materials as Tailored Nuclear Waste Forms: A Perspective. *Chemistry of Materials*, **2018**, 30, 4475-4488 | 9.6 | 69 |
| 150 | Grain Boundaries in Uranium Dioxide: Scanning Electron Microscopy Experiments and Atomistic Simulations. *Journal of the American Ceramic Society*, **2011**, 94, 1893-1900 | 3.8 | 66 |
| 149 | On the Thermodynamic Stability of Amorphous Intergranular Films in Covalent Materials. *Journal of the American Ceramic Society*, **1997**, 80, 717-732 | 3.8 | 61 |
| 148 | Atomistic simulations of copper oxidation and Cu/Cu2O interfaces using charge-optimized many-body potentials. *Physical Review B*, **2011**, 84, | 3.3 | 59 |
| 147 | Transition from thermal to athermal friction under cryogenic conditions. *Physical Review Letters*, **2009**, 102, 186102 | 7.4 | 58 |
| 146 | Atomistic Simulations of Materials Fracture and the Link between Atomic and Continuum Length Scales. *Journal of the American Ceramic Society*, **2005**, 81, 501-516 | 3.8 | 55 |
| 145 | Evaluation of computational techniques for solving the Boltzmann transport equation for lattice thermal conductivity calculations. *Physical Review B*, **2010**, 82, | 3.3 | 53 |

| | | | |
|---|---|---|---|
| 144 | Phonon Transport Simulator (PhonTS). *Computer Physics Communications*, **2015**, 192, 196-204 | 4.2 | 51 |
| 143 | Thermal Conductivity in Nanocrystalline Ceria Thin Films. *Journal of the American Ceramic Society*, **2014**, 97, 562-569 | 3.8 | 50 |
| 142 | Variable charge many-body interatomic potentials. *MRS Bulletin*, **2012**, 37, 504-512 | 3.2 | 48 |
| 141 | Thermal Transport in Off-Stoichiometric Uranium Dioxide by Atomic Level Simulation. *Journal of the American Ceramic Society*, **2009**, 92, 850-856 | 3.8 | 47 |
| 140 | Critical assessment of UO2 classical potentials for thermal conductivity calculations. *Journal of Materials Science*, **2012**, 47, 7693-7702 | 4.3 | 46 |
| 139 | Thermal conductance across grain boundaries in diamond from molecular dynamics simulation. *Journal of Applied Physics*, **2007**, 102, 063503 | 2.5 | 43 |
| 138 | Sliding orientation effects on the tribological properties of polytetrafluoroethylene. *Journal of Applied Physics*, **2007**, 102, 123509 | 2.5 | 43 |
| 137 | Thermodynamics and Electronic Properties of Heterometallic Multinuclear Actinide-Containing Metal-Organic Frameworks with "Structural Memory". *Journal of the American Chemical Society*, **2019**, 141, 11628-11640 | 16.4 | 42 |
| 136 | Molecular dynamics study of the adhesion of Cu/SiO2 interfaces using a variable-charge interatomic potential. *Physical Review B*, **2011**, 83, | 3.3 | 42 |
| 135 | Structure and energetics of ferroelectric domain walls in LiNbO3 from atomic-level simulations. *Physical Review B*, **2010**, 82, | 3.3 | 42 |
| 134 | Energetics of Oxidation in MoS2 Nanoparticles by Density Functional Theory. *Journal of Physical Chemistry C*, **2011**, 115, 10606-10616 | 3.8 | 42 |
| 133 | Mechanistic materials modeling for nuclear fuel performance. *Annals of Nuclear Energy*, **2017**, 105, 11-24 | 1.7 | 41 |
| 132 | Crossover in thermal transport properties of natural, perovskite-structured superlattices. *Applied Physics Letters*, **2009**, 95, 161906 | 3.4 | 41 |
| 131 | Nanoindentation of gold and gold alloys by molecular dynamics simulation. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2016**, 651, 346-357 | 5.3 | 39 |
| 130 | Fitting empirical potentials: Challenges and methodologies. *Current Opinion in Solid State and Materials Science*, **2013**, 17, 263-270 | 12 | 39 |
| 129 | A critical assessment of interatomic potentials for ceria with application to its elastic properties. *Solid State Ionics*, **2010**, 181, 551-556 | 3.3 | 39 |
| 128 | Effects of edge dislocations on thermal transport in UO2. *Journal of Nuclear Materials*, **2013**, 434, 203-209 | 3.3 | 38 |
| 127 | Stability and charge transfer levels of extrinsic defects in LiNbO3. *Physical Review B*, **2010**, 82, | 3.3 | 38 |

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|---|---|---|---|
| 126 | Phonon density of states and anharmonicity of UO2. *Physical Review B*, **2014**, 89, | 3.3 | 37 |
| 125 | Structure and energetics of 180° domain walls in PbTiO3 by density functional theory. *Journal of Physics Condensed Matter*, **2011**, 23, 175902 | 1.8 | 37 |
| 124 | Atomistic study of grain boundary sink strength under prolonged electron irradiation. *Journal of Nuclear Materials*, **2012**, 422, 69-76 | 3.3 | 36 |
| 123 | Vacancy-Ordered Structure of Cubic Bismuth Oxide from Simulation and Crystallographic Analysis. *Journal of the American Ceramic Society*, **2008**, 91, 2349-2356 | 3.8 | 36 |
| 122 | Kinetically evolving irradiation-induced point defect clusters in UO2 by molecular dynamics simulation. *Physical Review B*, **2009**, 80, | 3.3 | 35 |
| 121 | Molecular dynamics investigation of the lubrication mechanism of carbon nano-onions. *Computational Materials Science*, **2012**, 54, 91-96 | 3.2 | 33 |
| 120 | Structure and energetics of Er defects in LiNbO3 from first-principles and thermodynamic calculations. *Physical Review B*, **2009**, 80, | 3.3 | 33 |
| 119 | Entropy contributions to phase stability in binary random solid solutions. *Npj Computational Materials*, **2018**, 4, | 10.9 | 33 |
| 118 | Materials science. Simulating multifunctional structures. *Science*, **2009**, 325, 1634-5 | 33.3 | 32 |
| 117 | Thermal transport in polyethylene and at polyethylene-diamond interfaces investigated using molecular dynamics simulation. *Journal of Physics Condensed Matter*, **2009**, 21, 084219 | 1.8 | 31 |
| 116 | Microtubule nanospool formation by active self-assembly is not initiated by thermal activation. *Soft Matter*, **2011**, 7, 3108-3115 | 3.6 | 30 |
| 115 | Structure and diffusion of intrinsic defect complexes in LiNbO3 from density functional theory calculations. *Journal of Physics Condensed Matter*, **2010**, 22, 135002 | 1.8 | 30 |
| 114 | Stoichiometry of the LaFeO3 (010) surface determined from first-principles and thermodynamic calculations. *Physical Review B*, **2011**, 83, | 3.3 | 29 |
| 113 | Effect of the sliding orientation on the tribological properties of polyethylene in molecular dynamics simulations. *Journal of Applied Physics*, **2008**, 103, 083502 | 2.5 | 29 |
| 112 | Interfacial phonon scattering in semiconductor nanowires by molecular-dynamics simulation. *Journal of Applied Physics*, **2006**, 99, 123715 | 2.5 | 28 |
| 111 | Effects of Atomic-Level Disorder at Solid Interfaces. *MRS Bulletin*, **1990**, 15, 38-45 | 3.2 | 28 |
| 110 | Graphene-Titanium Interfaces from Molecular Dynamics Simulations. *ACS Applied Materials & Interfaces*, **2017**, 9, 33288-33297 | 9.5 | 27 |
| 109 | Atomic-Level Simulation of Ferroelectricity in Oxides: Current Status and Opportunities. *Annual Review of Materials Research*, **2007**, 37, 239-270 | 12.8 | 27 |

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|---|---|---|---|
| 108 | Homogeneous hydride formation path in □Zr: Molecular dynamics simulations with the charge-optimized many-body potential. *Acta Materialia*, **2016**, 111, 357-365 | 8.4 | 27 |
| 107 | Atomistic simulations of the adsorption and migration barriers of Cu adatoms on ZnO surfaces using COMB potentials. *Surface Science*, **2012**, 606, 1280-1288 | 1.8 | 26 |
| 106 | NSF cyberinfrastructures: A new paradigm for advancing materials simulation. *Current Opinion in Solid State and Materials Science*, **2013**, 17, 298-304 | 12 | 25 |
| 105 | The effect of normal load on polytetrafluoroethylene tribology. *Journal of Physics Condensed Matter*, **2009**, 21, 144201 | 1.8 | 25 |
| 104 | Grain-boundary source/sink behavior for point defects: An atomistic simulation study. *International Journal of Materials Research*, **2009**, 100, 550-555 | 0.5 | 25 |
| 103 | Thermal transport properties of MgO and Nd2Zr2O7 pyrochlore by molecular dynamics simulation. *Journal of Nuclear Materials*, **2008**, 380, 1-7 | 3.3 | 24 |
| 102 | Effect of Temperature on the Friction and Wear of PTFE by Atomic-Level Simulation. *Tribology Letters*, **2015**, 58, 1 | 2.8 | 23 |
| 101 | Impact of homogeneous strain on uranium vacancy diffusion in uranium dioxide. *Physical Review B*, **2015**, 91, | 3.3 | 23 |
| 100 | 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 | 3.3 | 23 |
| 99 | Data-Driven Model for Estimation of Friction Coefficient Via Informatics Methods. *Tribology Letters*, **2012**, 47, 211-221 | 2.8 | 23 |
| 98 | Nanoindentation of Zr by molecular dynamics simulation. *Journal of Nuclear Materials*, **2015**, 467, 742-757 | 3.3 | 22 |
| 97 | 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 | 3.3 | 22 |
| 96 | Phonon-mediated thermal transport: Confronting theory and microscopic simulation with experiment. *Current Opinion in Solid State and Materials Science*, **2013**, 17, 1-9 | 12 | 22 |
| 95 | 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 | 3.2 | 22 |
| 94 | Phonon-Mediated Thermal Conductivity in Ionic Solids by Lattice Dynamics-Based Methods. *Journal of the American Ceramic Society*, **2011**, 94, 3523-3531 | 3.8 | 22 |
| 93 | Optimized many body potential for fcc metals. *Philosophical Magazine Letters*, **2009**, 89, 136-144 | 1 | 22 |
| 92 | Deformation processes in polycrystalline Zr by molecular dynamics simulations. *Journal of Nuclear Materials*, **2015**, 462, 147-159 | 3.3 | 21 |
| 91 | Effect of inversion on thermoelastic and thermal transport properties of MgAl2O4 spinel by atomistic simulation. *Journal of Materials Science*, **2011**, 46, 55-62 | 4.3 | 21 |

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|---|---|---|---|
| 90 | Atomistic Simulations of Integranular Fracture in Symmetric-Tilt Grain Boundaries. *Journal of Materials Science*, **1999**, 7, 45-55 | | 21 |
| 89 | Properties of Ti/TiC Interfaces from Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2016**, 120, 12530-12538 | 3.8 | 21 |
| 88 | A charge optimized many-body (COMB) potential for titanium and titania. *Journal of Physics Condensed Matter*, **2014**, 26, 315007 | 1.8 | 20 |
| 87 | Charge-optimized many-body (COMB) potential for zirconium. *Journal of Nuclear Materials*, **2013**, 441, 274-279 | 3.3 | 20 |
| 86 | Influence of the Molecular Level Structure of Polyethylene and Polytetrafluoroethylene on Their Tribological Response. *Tribology Letters*, **2011**, 42, 193-201 | 2.8 | 20 |
| 85 | Metric for strong intrinsic fourth-order phonon anharmonicity. *Physical Review B*, **2017**, 95, | 3.3 | 19 |
| 84 | The role of charge and ionic radius on fission product segregation to a model UO2 grain boundary. *Journal of Applied Physics*, **2013**, 113, 134902 | 2.5 | 19 |
| 83 | Effect of ionic polarizability on oxygen diffusion in Bi2O3 from atomistic simulation. *Ionics*, **2010**, 16, 297-303 | 2.7 | 19 |
| 82 | Shape of ferroelectric domains in LiNbO3 and LiTaO3 from defect/domain-wall interactions. *Applied Physics Letters*, **2011**, 98, 092903 | 3.4 | 18 |
| 81 | Interfacial thermal conductivity: Insights from atomic level simulation. *Journal of Materials Science*, **2005**, 40, 3143-3148 | 4.3 | 18 |
| 80 | Cu cluster deposition on ZnO101□0: Morphology and growth mode predicted from molecular dynamics simulations. *Surface Science*, **2014**, 621, 109-116 | 1.8 | 16 |
| 79 | Local probing of the interaction between intrinsic defects and ferroelectric domain walls in lithium niobate. *Applied Physics Letters*, **2013**, 102, 042905 | 3.4 | 16 |
| 78 | Kinetically driven point-defect clustering in irradiated MgO by molecular-dynamics simulation. *Scripta Materialia*, **2009**, 60, 691-694 | 5.6 | 16 |
| 77 | Nanoindentation of ZrO2 and ZrO2/Zr systems by molecular dynamics simulation. *Journal of Nuclear Materials*, **2017**, 486, 250-266 | 3.3 | 15 |
| 76 | A charge-optimized many-body potential for the U-UO2-O2 system. *Journal of Physics Condensed Matter*, **2013**, 25, 505401 | 1.8 | 15 |
| 75 | Charge Optimized Many Body (COMB) potentials for simulation of nuclear fuel and clad. *Computational Materials Science*, **2018**, 148, 231-241 | 3.2 | 14 |
| 74 | Classical interatomic potential for orthorhombic uranium. *Journal of Physics Condensed Matter*, **2012**, 24, 235403 | 1.8 | 14 |
| 73 | Structure of Bi2O3 from density functional theory: A systematic crystallographic analysis. *Journal of Solid State Chemistry*, **2009**, 182, 1222-1228 | 3.3 | 14 |

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|---|---|---|---|
| 72 | Anisotropic thermal properties in orthorhombic perovskites. *Journal of Materials Science*, **2010**, 45, 168-176 | 4.5 | 14 |
| 71 | Atomic-level deformation of CuxZr100-x metallic glasses under shock loading. *Journal of Applied Physics*, **2018**, 123, 215101 | 2.5 | 14 |
| 70 | Anisotropy in oxidation of zirconium surfaces from density functional theory calculations. *Computational Materials Science*, **2015**, 98, 112-116 | 3.2 | 13 |
| 69 | 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 | 3.3 | 13 |
| 68 | Shock compression of Cu x Zr100 metallic glasses from molecular dynamics simulations. *Journal of Materials Science*, **2018**, 53, 5719-5732 | 4.3 | 13 |
| 67 | Dynamical properties of AlN nanostructures and heterogeneous interfaces predicted using COMB potentials. *Computational Materials Science*, **2016**, 113, 80-87 | 3.2 | 13 |
| 66 | Solubility and clustering of ruthenium fission products in uranium dioxide as determined by density functional theory. *Physical Review B*, **2012**, 85, | 3.3 | 13 |
| 65 | Stabilization Mechanisms of LaFeO3 (010) Surfaces Determined with First Principles Calculations. *Journal of the American Ceramic Society*, **2011**, 94, 1931-1939 | 3.8 | 13 |
| 64 | Grain Boundaries in Silicon from Zero Temperature through Melting. *Journal of the American Ceramic Society*, **1990**, 73, 933-937 | 3.8 | 13 |
| 63 | Effect of Surface Chemistry on Water Interaction with Cu(111). *Langmuir*, **2016**, 32, 8061-70 | 4 | 13 |
| 62 | Heterometallic Actinide-Containing Photoresponsive Metal-Organic Frameworks: Dynamic and Static Tuning of Electronic Properties. *Angewandte Chemie - International Edition*, **2021**, 60, 8072-8080 | 16.4 | 13 |
| 61 | 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 | 2.3 | 12 |
| 60 | Thermal conductivity of argon at high pressure from first principles calculations. *Journal of Applied Physics*, **2013**, 114, 064902 | 2.5 | 12 |
| 59 | Thermal conductivity of UO2 fuel: Predicting fuel performance from simulation. *Jom*, **2011**, 63, 73-79 | 2.1 | 12 |
| 58 | Order-disorder behavior in KNbO3 and KNbO3/KTaO3 solid solutions and superlattices by molecular-dynamics simulation. *Journal of Materials Science*, **2005**, 40, 3213-3217 | 4.3 | 12 |
| 57 | Adhesion and diffusion at TiN/TiO2 interfaces: A first principles study. *Computational Materials Science*, **2017**, 130, 249-256 | 3.2 | 11 |
| 56 | Potential Optimization Software for Materials (POSMat). *Computer Physics Communications*, **2016**, 203, 201-211 | 4.2 | 11 |
| 55 | Morphology and growth modes of metal-oxides deposited on SrTiO3. *Surface Science*, **2009**, 603, 873-880 | 1.8 | 11 |

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|---|---|---|---|
| 54 | Introduction to thermal transport. *Materials Today*, **2005**, 8, 18-20 | 21.8 | 11 |
| 53 | Galvanic Replacement-Driven Transformations of Atomically Intermixed Bimetallic Colloidal Nanocrystals: Effects of Compositional Stoichiometry and Structural Ordering. *Langmuir*, **2018**, 34, 4340-4350 | 4 | 10 |
| 52 | Anharmonic properties in Mg2X (X=C,Si,Ge,Sn,Pb) from first-principles calculations. *Physical Review B*, **2015**, 92, | 3.3 | 10 |
| 51 | Effect of simulation conditions on friction in polytetrafluoroethylene (PTFE). *Journal of Computer-Aided Materials Design*, **2007**, 14, 239-246 | | 10 |
| 50 | Linking atomistic and mesoscale simulations of nanocrystalline materials: quantitative validation for the case of grain growth. *Philosophical Magazine*, **2003**, 83, 3643-3659 | 1.6 | 10 |
| 49 | Surface diffusion on SrTiO3 (100): A temperature accelerated dynamics and first principles study. *Surface Science*, **2013**, 617, 237-241 | 1.8 | 9 |
| 48 | Computational discovery of lanthanide doped and Co-doped Y3Al5O12 for optoelectronic applications. *Applied Physics Letters*, **2015**, 107, 112109 | 3.4 | 9 |
| 47 | Interatomic potential for the structure and energetics of tetrahedrally coordinated silica polymorphs. *Physical Review B*, **2007**, 75, | 3.3 | 9 |
| 46 | Lattice expansion by intrinsic defects in uranium by molecular dynamics simulation. *Journal of Nuclear Materials*, **2016**, 475, 6-18 | 3.3 | 8 |
| 45 | Segregation of ruthenium to edge dislocations in uranium dioxide. *Journal of Nuclear Materials*, **2013**, 441, 96-102 | 3.3 | 8 |
| 44 | Void collapse and subsequent spallation in Cu50Zr50 metallic glass under shock loading by molecular dynamics simulations. *Journal of Applied Physics*, **2019**, 125, 215903 | 2.5 | 7 |
| 43 | Charge optimized many-body (COMB) potential for Al2O3 materials, interfaces, and nanostructures. *Journal of Physics Condensed Matter*, **2015**, 27, 305004 | 1.8 | 7 |
| 42 | Electronic structures and magnetism of Zr-, Th-, and U-based metal-organic frameworks (MOFs) by density functional theory. *Computational Materials Science*, **2020**, 184, 109903 | 3.2 | 7 |
| 41 | A Mechanism for TiO2 Formation on Stepped TiN(001) from First-Principles Calculations. *Journal of Physical Chemistry C*, **2014**, 118, 384-388 | 3.8 | 7 |
| 40 | Interaction between voids and grain boundaries in UO2 by molecular-dynamics simulation. *Journal of Nuclear Materials*, **2014**, 448, 53-61 | 3.3 | 7 |
| 39 | Design of Low Wear Polymer Composites. *Tribology Letters*, **2012**, 45, 79-87 | 2.8 | 7 |
| 38 | A third-generation charge optimized many body (COMB3) potential for nitrogen-containing organic molecules. *Computational Materials Science*, **2017**, 139, 153-161 | 3.2 | 7 |
| 37 | 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 | 0.3 | 7 |

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|---|---|---|---|
| 36 | Effect of fluorocarbon molecules confined between sliding self-mated PTFE surfaces. *Langmuir*, **2011**, 27, 9910-9 | 4 | 7 |
| 35 | Crossover in thermal transport mechanism in nanocrystalline silicon. *Applied Physics Letters*, **2006**, 88, 141908 | 3.4 | 7 |
| 34 | Elastic and thermal properties of hexagonal perovskites. *Computational Materials Science*, **2016**, 122, 139-145 | 3.2 | 7 |
| 33 | The Conundrum of Relaxation Volumes in First-Principles Calculations of Charged Defects in UO2. *Applied Sciences (Switzerland)*, **2019**, 9, 5276 | 2.6 | 7 |
| 32 | Generation and characterization of an improved carbon fiber model by molecular dynamics. *Carbon*, **2021**, 173, 232-244 | 10.4 | 7 |
| 31 | Toward an Atomistically Informed Fuel Performance Code: Thermal Properties Using FRAPCON and Molecular Dynamics Simulation. *Nuclear Technology*, **2009**, 165, 308-312 | 1.4 | 6 |
| 30 | Depinning of the ferroelectric domain wall in congruent LiNbO3. *Applied Physics Letters*, **2016**, 109, 082905 | 3.4 | 6 |
| 29 | Heterometallic multinuclear nodes directing MOF electronic behavior. *Chemical Science*, **2020**, 11, 7379-7389 | 9.1 | 5 |
| 28 | Sequestration of Radionuclides in Metal–Organic Frameworks from Density Functional Theory Calculations. *Journal of Physical Chemistry C*, **2019**, 123, 26842-26855 | 3.8 | 5 |
| 27 | Charge optimized many-body potential for aluminum. *Journal of Physics Condensed Matter*, **2015**, 27, 015003 | 1.8 | 5 |
| 26 | Effect of the initial temperature on the shock response of Cu50Zr50 bulk metallic glass by molecular dynamics simulation. *Journal of Applied Physics*, **2021**, 129, 165103 | 2.5 | 5 |
| 25 | Charge optimized many-body (COMB) potential for dynamical simulation of Ni-Al phases. *Journal of Physics Condensed Matter*, **2015**, 27, 336302 | 1.8 | 4 |
| 24 | Overcoming the Interfacial Lattice Mismatch: Geometry Control of Gold–Nickel Bimetallic Heteronanostructures. *Particle and Particle Systems Characterization*, **2018**, 35, 1700361 | 3.1 | 4 |
| 23 | Titanium-Carbide Formation at Defective Curved Graphene-Titanium Interfaces. *MRS Advances*, **2018**, 3, 457-462 | 0.7 | 4 |
| 22 | Molecular dynamics simulations of SrTiO3 thin-film growth from cluster deposition. *Journal of Physics Condensed Matter*, **2010**, 22, 045001 | 1.8 | 4 |
| 21 | Thermal conductivity of the n = 1, 5 and 10 members of the (SrTiO3)nSrO Ruddlesden–Popper superlattices. *Applied Physics Letters*, **2021**, 118, 091904 | 3.4 | 4 |
| 20 | Publisher's Note: Second-generation charge-optimized many-body potential for Si/SiO2 and amorphous silica [Phys. Rev. B 82, 235302 (2010)]. *Physical Review B*, **2010**, 82, | 3.3 | 3 |
| 19 | Molecular dynamics simulation of the shock response of materials: A tutorial. *Journal of Applied Physics*, **2022**, 131, 051101 | 2.5 | 3 |

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|---|---|---|---|
| 18 | The influence of alloying on the stacking fault energy of gold from density functional theory calculations. *Computational Materials Science*, **2021**, 188, 110236 | 3.2 | 3 |
| 17 | Heterometallic Actinide-Containing Photoresponsive Metal-Organic Frameworks: Dynamic and Static Tuning of Electronic Properties. *Angewandte Chemie*, **2021**, 133, 8152-8160 | 3.6 | 3 |
| 16 | High-temperature oxidation of carbon fiber and char by molecular dynamics simulation. *Carbon*, **2021**, 185, 449-463 | 10.4 | 3 |
| 15 | Thermodynamics and kinetics of ordered and disordered Cu/Au alloys from first principles calculations. *Journal of Alloys and Compounds*, **2019**, 809, 151615 | 5.7 | 2 |
| 14 | 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 | 1.2 | 2 |
| 13 | Role of electronic effects on the incorporation of Cr at a Σ5 grain boundary in UO2. *Computational Materials Science*, **2013**, 78, 29-33 | 3.2 | 2 |
| 12 | A computational study of SrTiO3 thin film deposition: Morphology and growth modes. *Journal of Materials Research*, **2009**, 24, 1994-2000 | 2.5 | 2 |
| 11 | Modeling reaction pathways of low energy particle deposition on thiophene via ab initio calculations. *Chemical Physics Letters*, **2011**, 510, 197-201 | 2.5 | 2 |
| 10 | Interactions of Defects and Domain Walls in LiNbO3：Insights from Simulations. *IOP Conference Series: Materials Science and Engineering*, **2010**, 15, 012003 | 0.4 | 2 |
| 9 | Dynamics of graphene/Al interfaces using COMB3 potentials. *Physical Review Materials*, **2019**, 3, | 3.2 | 2 |
| 8 | Zhao et al. Reply:. *Physical Review Letters*, **2010**, 105, | 7.4 | 1 |
| 7 | Phase-field modeling of carbon fiber oxidation coupled with heat conduction. *Computational Materials Science*, **2022**, 204, 111156 | 3.2 | 1 |
| 6 | Lattice stability and point defect energetics of TiSi2 and TiGe2 allotropes from first-principles calculations. *Journal of Applied Physics*, **2021**, 129, 085104 | 2.5 | 1 |
| 5 | Lattice thermal conductivity of quartz at high pressure and temperature from the Boltzmann transport equation. *Journal of Applied Physics*, **2019**, 126, 215106 | 2.5 | 0 |
| 4 | Stability of epitaxial pseudocubic group IV-V semiconductors. *Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics*, **2019**, 37, 050602 | 1.3 | |
| 3 | Role of cyberinfrastructure in educating the next generation of computational materials scientists. *Integrating Materials and Manufacturing Innovation*, **2014**, 3, 85-89 | 2.9 | |
| 2 | 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 | 2.5 | |
| 1 | Nanoindentation of ZrH2 by molecular dynamics simulation. *Journal of Nuclear Materials*, **2020**, 540, 152391 | 3.1 | |