Susan B Sinnott

List of Publications by Year in Descending Order

272 papers	12,501 citations	53 h-index	103 g-index
290 ext. papers	13,574 ext. citations	4.3 avg, IF	6.44 L-index

#	Paper	IF	Citations
272	Surface reconstruction of oxidized platinum nanoparticles using classical molecular dynamics simulations. *Computational Materials Science*, **2022**, 209, 111364	3.2	0
271	Single-Step Direct Laser Writing of Multimetal Oxygen Evolution Catalysts from Liquid Precursors. *ACS Nano*, **2021**, 15, 9796-9807	16.7	4
270	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
269	Optimized utilization of COMB3 reactive potentials in LAMMPS. *Journal of Chemical Physics*, **2020**, 152, 224702	3.9	3
268	Multiscale computational understanding and growth of 2D materials: a review. *Npj Computational Materials*, **2020**, 6,	10.9	49
267	Influence of phase and interface properties on the stress state dependent fracture initiation behavior in DP steels through computational modeling. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2020**, 776, 138981	5.3	5
266	Effects of surface charge and cluster size on the electrochemical dissolution of platinum nanoparticles using COMB3 and continuum electrolyte models. *Journal of Chemical Physics*, **2020**, 152, 064102	3.9	1
265	Density Functional Theory Study of Epitaxially Strained Monolayer Transition Metal Chalcogenides for Piezoelectricity Generation. *ACS Applied Nano Materials*, **2020**, 3, 384-390	5.6	7
264	Superconductivity enhancement in phase-engineered molybdenum carbide/disulfide vertical heterostructures. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 19685-19693	11.5	4
263	Carbon doping of WS monolayers: Bandgap reduction and p-type doping transport. *Science Advances*, **2019**, 5, eaav5003	14.3	70
262	Large tetragonality and room temperature ferroelectricity in compressively strained CaTiO3 thin films. *APL Materials*, **2019**, 7, 051104	5.7	5
261	Multi-Step Topochemical Pathway to Metastable MoAlB and Related Two-Dimensional Nanosheet Heterostructures. *Journal of the American Chemical Society*, **2019**, 141, 10852-10861	16.4	43
260	Effects of water on the mechanical properties of silica glass using molecular dynamics. *Acta Materialia*, **2019**, 178, 36-44	8.4	12
259	Data-driven glass/ceramic science research: Insights from the glass and ceramic and data science/informatics communities. *Journal of the American Ceramic Society*, **2019**, 102, 6385-6406	3.8	12
258	The structure of graphene on graphene/C/Cu interfaces: a molecular dynamics study. *Nanotechnology*, **2019**, 30, 505707	3.4	5
257	Dynamics of graphene/Al interfaces using COMB3 potentials. *Physical Review Materials*, **2019**, 3,	3.2	2
256	Predicting the Electrochemical Synthesis of 2D Materials from First Principles. *Journal of Physical Chemistry C*, **2019**, 123, 3180-3187	3.8	18

255	Charge Optimized Many Body (COMB) potentials for simulation of nuclear fuel and clad. *Computational Materials Science*, **2018**, 148, 231-241	3.2	14
254	Titanium-Carbide Formation at Defective Curved Graphene-Titanium Interfaces. *MRS Advances*, **2018**, 3, 457-462	0.7	4
253	Applied Potentials in Variable-Charge Reactive Force Fields for Electrochemical Systems. *Journal of Physical Chemistry A*, **2018**, 122, 631-638	2.8	11
252	Strain effects on domain structures in ferroelectric thin films from phase-field simulations. *Journal of the American Ceramic Society*, **2018**, 101, 4783-4790	3.8	6
251	Molecular Simulation of Capture of Sulfur-Containing Gases by Porous Aromatic Frameworks. *Journal of Physical Chemistry C*, **2018**, 122, 18456-18467	3.8	15
250	Development of a ReaxFF Reactive Force Field for NaSiOx/Water Systems and Its Application to Sodium and Proton Self-Diffusion. *Journal of Physical Chemistry C*, **2018**, 122, 19613-19624	3.8	41
249	High-throughput density functional calculations to optimize properties and interfacial chemistry of piezoelectric materials. *Physical Review Materials*, **2018**, 2,	3.2	1
248	Discovering chemical site occupancy- modulus correlations in Ni based intermetallics via statistical learning methods. *Computational Condensed Matter*, **2018**, 14, 8-14	1.7	1
247	Three-dimensional atomic scale electron density reconstruction of octahedral tilt epitaxy in functional perovskites. *Nature Communications*, **2018**, 9, 5220	17.4	18
246	Transformation of 2D group-III selenides to ultra-thin nitrides: enabling epitaxy on amorphous substrates. *Nanotechnology*, **2018**, 29, 47LT02	3.4	6
245	Nanoscale Structure and Dynamics of Water on Pt and Cu Surfaces from MD Simulations. *Langmuir*, **2018**, 34, 11905-11911	4	10
244	Nanoindentation of ZrO2 and ZrO2/Zr systems by molecular dynamics simulation. *Journal of Nuclear Materials*, **2017**, 486, 250-266	3.3	15
243	Topology-Scaling Identification of Layered Solids and Stable Exfoliated 2D Materials. *Physical Review Letters*, **2017**, 118, 106101	7.4	193
242	Adhesion and diffusion at TiN/TiO2 interfaces: A first principles study. *Computational Materials Science*, **2017**, 130, 249-256	3.2	11
241	Charge optimized many body (COMB) potentials for Pt and Au. *Journal of Physics Condensed Matter*, **2017**, 29, 225901	1.8	9
240	On the Multiple Event Detection in Atom Probe Tomography. *Microscopy and Microanalysis*, **2017**, 23, 618-619	0.5	11
239	Computational Study of Low Interlayer Friction in TiC (n = 1, 2, and 3) MXene. *ACS Applied Materials & Interfaces*, **2017**, 9, 34467-34479	9.5	62
238	Graphene-Titanium Interfaces from Molecular Dynamics Simulations. *ACS Applied Materials & Interfaces*, **2017**, 9, 33288-33297	9.5	27

237	Two-Dimensional Intrinsic Half-Metals With Large Spin Gaps. *Nano Letters*, **2017**, 17, 5251-5257	11.5	111
236	A third-generation charge optimized many body (COMB3) potential for nitrogen-containing organic molecules. *Computational Materials Science*, **2017**, 139, 153-161	3.2	7
235	Computer Simulations of Nanometer-Scale Indentation and Friction. *Springer Handbooks*, **2017**, 1013-1067	13	
234	Computational investigation on CO2 adsorption in titanium carbide-derived carbons with residual titanium. *Carbon*, **2017**, 111, 741-751	10.4	9
233	Computer Simulations of Nanometer-Scale Indentation and Friction **2017**, 301-370		1
232	Computational discovery of stable M2AX phases. *Physical Review B*, **2016**, 94,	3.3	50
231	MPInterfaces: A Materials Project based Python tool for high-throughput computational screening of interfacial systems. *Computational Materials Science*, **2016**, 122, 183-190	3.2	72
230	Behavior of molecules and molecular ions near a field emitter. *New Journal of Physics*, **2016**, 18, 033031	2.9	104
229	Dynamical properties of AlN nanostructures and heterogeneous interfaces predicted using COMB potentials. *Computational Materials Science*, **2016**, 113, 80-87	3.2	13
228	Probing the accuracy of reactive and non-reactive force fields to describe physical and chemical properties of graphene-oxide. *Computational Materials Science*, **2016**, 114, 236-243	3.2	19
227	Lattice expansion by intrinsic defects in uranium by molecular dynamics simulation. *Journal of Nuclear Materials*, **2016**, 475, 6-18	3.3	8
226	Potential Optimization Software for Materials (POSMat). *Computer Physics Communications*, **2016**, 203, 201-211	4.2	11
225	Predicted Surface Composition and Thermodynamic Stability of MXenes in Solution. *Journal of Physical Chemistry C*, **2016**, 120, 3550-3556	3.8	143
224	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
223	Thermal transport at (001) twist grain boundaries in UO2. *Journal of Nuclear Materials*, **2016**, 479, 167-173	3.3	5
222	Role of composition and structure on the properties of metal/multifunctional ceramic interfaces. *Journal of Applied Physics*, **2016**, 120, 045310	2.5	6
221	Computational characterization of lightweight multilayer MXene Li-ion battery anodes. *Applied Physics Letters*, **2016**, 108, 023901	3.4	66
220	Computational discovery and characterization of polymorphic two-dimensional IVV materials. *Applied Physics Letters*, **2016**, 109, 192103	3.4	41

219	Diffusion Across M/Pb(Zr,Ti)O3 Interfaces (M=Pt3Pb or Pt) Under Different System Conditions. *Journal of the American Ceramic Society*, **2016**, 99, 356-362	3.8	2
218	Properties of Ti/TiC Interfaces from Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2016**, 120, 12530-12538	3.8	21
217	Effect of Surface Chemistry on Water Interaction with Cu(111). *Langmuir*, **2016**, 32, 8061-70	4	13
216	Charge optimized many-body (COMB) potential for dynamical simulation of Ni-Al phases. *Journal of Physics Condensed Matter*, **2015**, 27, 336302	1.8	4
215	Charge optimized many-body (COMB) potential for Al2O3 materials, interfaces, and nanostructures. *Journal of Physics Condensed Matter*, **2015**, 27, 305004	1.8	7
214	Effect of Temperature on the Friction and Wear of PTFE by Atomic-Level Simulation. *Tribology Letters*, **2015**, 58, 1	2.8	23
213	Deformation processes in polycrystalline Zr by molecular dynamics simulations. *Journal of Nuclear Materials*, **2015**, 462, 147-159	3.3	21
212	Nanoindentation of Zr by molecular dynamics simulation. *Journal of Nuclear Materials*, **2015**, 467, 742-757	3.3	22
211	Anisotropy in oxidation of zirconium surfaces from density functional theory calculations. *Computational Materials Science*, **2015**, 98, 112-116	3.2	13
210	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
209	Mapping Chemical Selection Pathways for Designing Multicomponent Alloys: an informatics framework for materials design. *Scientific Reports*, **2015**, 5, 17960	4.9	20
208	Direct Observation of Chemical Pressure in Intermetallic Alloys by Scanning Transmission Electron Microscopy. *Microscopy and Microanalysis*, **2015**, 21, 1519-1520	0.5	
207	Computational discovery of lanthanide doped and Co-doped Y3Al5O12 for optoelectronic applications. *Applied Physics Letters*, **2015**, 107, 112109	3.4	9
206	Combined Experimental and Computational Methods Reveal the Evolution of Buried Interfaces during Synthesis of Ferroelectric Thin Films. *Advanced Materials Interfaces*, **2015**, 2, 1500181	4.6	11
205	Charge optimized many-body potential for aluminum. *Journal of Physics Condensed Matter*, **2015**, 27, 015003	1.8	5
204	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
203	Molecular dynamics simulations of CO2 reduction on Cu(111) and Cu/ZnO(10 1□0) using charge optimized many body potentials. *Catalysis Communications*, **2014**, 52, 84-87	3.2	21
202	Cu cluster deposition on ZnO101□0: Morphology and growth mode predicted from molecular dynamics simulations. *Surface Science*, **2014**, 621, 109-116	1.8	16

201	A charge optimized many-body potential for titanium nitride (TiN). *Journal of Physics Condensed Matter*, **2014**, 26, 265004	1.8	8
200	Synthesis, Characterization, and Computation of Catalysts at the Center for Atomic-Level Catalyst Design. *Journal of Physical Chemistry C*, **2014**, 118, 20043-20069	3.8	17
199	Defect Engineering of BiI3 Single Crystals: Enhanced Electrical and Radiation Performance for Room Temperature Gamma-Ray Detection. *Journal of Physical Chemistry C*, **2014**, 118, 3244-3250	3.8	59
198	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
197	A charge optimized many-body (COMB) potential for titanium and titania. *Journal of Physics Condensed Matter*, **2014**, 26, 315007	1.8	20
196	Interaction between voids and grain boundaries in UO2 by molecular-dynamics simulation. *Journal of Nuclear Materials*, **2014**, 448, 53-61	3.3	7
195	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
194	Direct Lattice Parameter Measurements Using HAADF-STEM. *Microscopy and Microanalysis*, **2014**, 20, 1050-1051	0.5	
193	Role of cyberinfrastructure in educating the next generation of computational materials scientists. *Integrating Materials and Manufacturing Innovation*, **2014**, 3, 85-89	2.9	
192	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
191	Growth and Structure of Cu and Au on the Nonpolar ZnO(101 0) Surface: STM, XPS, and DFT Studies. *Journal of Physical Chemistry C*, **2013**, 117, 18386-18397	3.8	24
190	Surface diffusion on SrTiO3 (100): A temperature accelerated dynamics and first principles study. *Surface Science*, **2013**, 617, 237-241	1.8	9
189	Fitting empirical potentials: Challenges and methodologies. *Current Opinion in Solid State and Materials Science*, **2013**, 17, 263-270	12	39
188	Mechanisms for hyperthermal polyatomic hydrocarbon modification of PMMA surfaces from molecular dynamics simulations. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2013**, 31, 061403	2.9	
187	NSF cyberinfrastructures: A new paradigm for advancing materials simulation. *Current Opinion in Solid State and Materials Science*, **2013**, 17, 298-304	12	25
186	Effects of edge dislocations on thermal transport in UO2. *Journal of Nuclear Materials*, **2013**, 434, 203-209	3.3	38
185	Charge-optimized many-body (COMB) potential for zirconium. *Journal of Nuclear Materials*, **2013**, 441, 274-279	3.3	20
184	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

183	Segregation of ruthenium to edge dislocations in uranium dioxide. *Journal of Nuclear Materials*, **2013**, 441, 96-102	3.3	8
182	Atomic-Scale Quantification of the Chemical Modification of Polystyrene through S, SC, and SH Deposition from Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2013**, 117, 12103-12110	3.8	1
181	Reactive Potentials for Advanced Atomistic Simulations. *Annual Review of Materials Research*, **2013**, 43, 109-129	12.8	147
180	A charge-optimized many-body potential for the U-UO2-O2 system. *Journal of Physics Condensed Matter*, **2013**, 25, 505401	1.8	15
179	Structural effects on mechanical response of MoS2 nanostructures during compression. *Journal of Applied Physics*, **2013**, 114, 034308	2.5	7
178	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
177	Material design and discovery with computational materials science. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2013**, 31, 050812	2.9	12
176	Computational investigation of the mechanical and tribological responses of amorphous carbon nanoparticles. *Journal of Applied Physics*, **2013**, 113, 073509	2.5	4
175	Design of Low Wear Polymer Composites. *Tribology Letters*, **2012**, 45, 79-87	2.8	7
174	Variable charge many-body interatomic potentials. *MRS Bulletin*, **2012**, 37, 504-512	3.2	48
173	Primary radiation defect production in polyethylene and cellulose. *Journal of Physical Chemistry B*, **2012**, 116, 13932-8	3.4	18
172	Acetylene Ion Enhanced Bonding of PbS Nanoparticles to Quaterthiophene in Thin Films. *Journal of Physical Chemistry C*, **2012**, 116, 21693-21698	3.8	3
171	Variable charge reactive potential for hydrocarbons to simulate organic-copper interactions. *Journal of Physical Chemistry A*, **2012**, 116, 7976-91	2.8	76
170	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
169	Critical assessment of UO2 classical potentials for thermal conductivity calculations. *Journal of Materials Science*, **2012**, 47, 7693-7702	4.3	46
168	Molecular dynamics investigation of the lubrication mechanism of carbon nano-onions. *Computational Materials Science*, **2012**, 54, 91-96	3.2	33
167	Three decades of many-body potentials in materials research. *MRS Bulletin*, **2012**, 37, 469-473	3.2	39
166	Mechanical behavior of MoS2 nanotubes under compression, tension, and torsion from molecular dynamics simulations. *Journal of Applied Physics*, **2012**, 112, 123510	2.5	36

165	Lubrication mechanisms of hollow-core inorganic fullerene-like nanoparticles: coupling experimental and computational works. *Nanotechnology*, **2012**, 23, 375701	3.4	38
164	Solubility and clustering of ruthenium fission products in uranium dioxide as determined by density functional theory. *Physical Review B*, **2012**, 85,	3.3	13
163	Hyperthermal Atomic Oxygen and Argon Modification of Polymer Surfaces Investigated by Molecular Dynamics Simulations. *Plasma Processes and Polymers*, **2012**, 9, 690-700	3.4	8
162	Classical interatomic potential for orthorhombic uranium. *Journal of Physics Condensed Matter*, **2012**, 24, 235403	1.8	14
161	Friction and Wear of Pyrophyllite on the Atomic Scale. *Tribology Letters*, **2012**, 46, 159-165	2.8	7
160	Data-Driven Model for Estimation of Friction Coefficient Via Informatics Methods. *Tribology Letters*, **2012**, 47, 211-221	2.8	23
159	Predicted mechanical properties of a coiled carbon nanotube. *Carbon*, **2012**, 50, 968-976	10.4	35
158	Computer Simulations of Nanometer-Scale Indentation and Friction **2011**, 439-525		4
157	Molecular dynamics study of the adhesion of Cu/SiO2 interfaces using a variable-charge interatomic potential. *Physical Review B*, **2011**, 83,	3.3	42
156	Stoichiometry of the LaFeO3 (010) surface determined from first-principles and thermodynamic calculations. *Physical Review B*, **2011**, 83,	3.3	29
155	Segregation of xenon to dislocations and grain boundaries in uranium dioxide. *Physical Review B*, **2011**, 84,	3.3	46
154	Atomistic simulations of copper oxidation and Cu/Cu2O interfaces using charge-optimized many-body potentials. *Physical Review B*, **2011**, 84,	3.3	59
153	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
152	Stabilization Mechanisms of LaFeO3 (010) Surfaces Determined with First Principles Calculations. *Journal of the American Ceramic Society*, **2011**, 94, 1931-1939	3.8	13
151	Reparameterization of the REBO-CHO potential for graphene oxide molecular dynamics simulations. *Physical Review B*, **2011**, 84,	3.3	29
150	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
149	Influence of the Molecular Level Structure of Polyethylene and Polytetrafluoroethylene on Their Tribological Response. *Tribology Letters*, **2011**, 42, 193-201	2.8	20
148	Mechanisms of Ion-Beam Modification of Terthiophene Oligomers from Atomistic Simulations. *Journal of Physical Chemistry C*, **2011**, 115, 23936-23945	3.8	5

147	Effect of fluorocarbon molecules confined between sliding self-mated PTFE surfaces. *Langmuir*, **2011**, 27, 9910-9	4	7
146	Energetics of Oxidation in MoS2 Nanoparticles by Density Functional Theory. *Journal of Physical Chemistry C*, **2011**, 115, 10606-10616	3.8	42
145	Modeling reaction pathways of low energy particle deposition on polymer surfaces via first principle calculations. *Journal of Physical Chemistry A*, **2011**, 115, 4976-87	2.8	1
144	Modeling reaction pathways of low energy particle deposition on thiophene via ab initio calculations. *Chemical Physics Letters*, **2011**, 510, 197-201	2.5	2
143	Structure and energetics of 180° domain walls in PbTiO3 by density functional theory. *Journal of Physics Condensed Matter*, **2011**, 23, 175902	1.8	37
142	Zhao et al. Reply:. *Physical Review Letters*, **2010**, 105,	7.4	1
141	Molecular dynamics simulations of SrTiO3 thin-film growth from cluster deposition. *Journal of Physics Condensed Matter*, **2010**, 22, 045001	1.8	4
140	Multilevel Computational Analysis of Fluorocarbon Polyatomic Deposition on Diamond. *Journal of Physical Chemistry C*, **2010**, 114, 12535-12544	3.8	2
139	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
138	Intrinsic electrostatic effects in nanostructured ceramics. *Physical Review B*, **2010**, 81,	3.3	20
137	Charge-optimized many-body potential for the hafnium/hafnium oxide system. *Physical Review B*, **2010**, 81,	3.3	109
136	Second-generation charge-optimized many-body potential for Si/SiO2 and amorphous silica. *Physical Review B*, **2010**, 82,	3.3	79
135	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
134	Computer Simulations of Nanometer-Scale Indentation and Friction **2010**, 955-1011		2
133	Stability and charge transfer levels of extrinsic defects in LiNbO3. *Physical Review B*, **2010**, 82,	3.3	38
132	Interactions of Defects and Domain Walls in LiNbO3: Insights from Simulations. *IOP Conference Series: Materials Science and Engineering*, **2010**, 15, 012003	0.4	2
131	Effect of ionic polarizability on oxygen diffusion in δ-Bi2O3 from atomistic simulation. *Ionics*, **2010**, 16, 297-303	2.7	19
130	Friction Properties of Carbon Nano-Onions from Experiment and Computer Simulations. *Tribology Letters*, **2010**, 37, 75-81	2.8	64

129	Nanoindentation of surfactant aggregates. *Journal of Colloid and Interface Science*, **2010**, 349, 196-204	9.3	3
128	Amorphization of □-quartz and comparative study of defects in amorphized quartz and Si nanocrystals embedded in amorphous silica. *Nuclear Instruments & Methods in Physics Research B*, **2010**, 268, 3095-3098	1.2	1
127	A critical assessment of interatomic potentials for ceria with application to its elastic properties. *Solid State Ionics*, **2010**, 181, 551-556	3.3	39
126	Unique buckling responses of multi-walled carbon nanotubes incorporated as torsion springs. *Carbon*, **2010**, 48, 1697-1701	10.4	16
125	Atomic-Scale Simulations of the Mechanical Behavior of Carbon Nanotube Systems. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 255-295	0.7	2
124	A torsional parametric oscillator based on carbon nanotubes. *Applied Physics Letters*, **2009**, 95, 083112	3.4	9
123	Structure and energetics of Er defects in LiNbO3 from first-principles and thermodynamic calculations. *Physical Review B*, **2009**, 80,	3.3	33
122	Transition from thermal to athermal friction under cryogenic conditions. *Physical Review Letters*, **2009**, 102, 186102	7.4	58
121	Publisher's Note: Mixed Bloch-Néel-Ising character of 180° ferroelectric domain walls [Phys. Rev. B 80, 060102 (2009)]. *Physical Review B*, **2009**, 80,	3.3	14
120	Mixed Bloch-Néel-Ising character of 180° ferroelectric domain walls. *Physical Review B*, **2009**, 80,	3.3	121
119	A computational study of SrTiO3 thin film deposition: Morphology and growth modes. *Journal of Materials Research*, **2009**, 24, 1994-2000	2.5	2
118	Computational and experimental studies of phase separation in pentacene:C60 mixtures. *Journal of Vacuum Science & Technology B*, **2009**, 27, 169		19
117	The effect of normal load on polytetrafluoroethylene tribology. *Journal of Physics Condensed Matter*, **2009**, 21, 144201	1.8	25
116	Piecewise-stationary bandit problems with side observations **2009**,		18
115	Morphology and growth modes of metal-oxides deposited on SrTiO3. *Surface Science*, **2009**, 603, 873-880	1.8	11
114	Thermal Transport in Off-Stoichiometric Uranium Dioxide by Atomic Level Simulation. *Journal of the American Ceramic Society*, **2009**, 92, 850-856	3.8	47
113	Modification of poly(methyl methacrylate) by keV Ar deposition. *Nuclear Instruments & Methods in Physics Research B*, **2009**, 267, 2525-2531	1.2	9
112	Energetics of intrinsic point defects in uranium dioxide from electronic-structure calculations. *Journal of Nuclear Materials*, **2009**, 384, 61-69	3.3	118

111	Structure of Bi2O3 from density functional theory: A systematic crystallographic analysis. *Journal of Solid State Chemistry*, **2009**, 182, 1222-1228	3.3	14
110	Energetics of charged point defects in rutile TiO2 by density functional theory. *Acta Materialia*, **2009**, 57, 5882-5891	8.4	29
109	Chemical Modification of Polypropylene and Polystyrene through Fluorocarbon Ion Beam Deposition. *Journal of Physical Chemistry C*, **2009**, 113, 17860-17865	3.8	2
108	Parametrization of a reactive many-body potential for Mo S systems. *Physical Review B*, **2009**, 79,	3.3	198
107	Thermodynamics of fission products in UO(2 − x). *Journal of Physics Condensed Matter*, **2009**, 21, 435602	1.8	45
106	Materials science. Simulating multifunctional structures. *Science*, **2009**, 325, 1634-5	33.3	32
105	Computational investigation of the mechanical properties of nanomaterials. *Diamond and Related Materials*, **2009**, 18, 438-442	3.5	6
104	Toward an Atomistically Informed Fuel Performance Code: Thermal Properties Using FRAPCON and Molecular Dynamics Simulation. *Nuclear Technology*, **2009**, 165, 308-312	1.4	6
103	Stability of intrinsic defects and defect clusters in LiNbO3 from density functional theory calculations. *Physical Review B*, **2008**, 78,	3.3	96
102	Coupling of surface relaxation and polarization in PbTiO3from atomistic simulation. *Journal of Physics Condensed Matter*, **2008**, 20, 395004	1.8	11
101	Integrating experimental and simulation length and time scales in mechanistic studies of friction. *Journal of Physics Condensed Matter*, **2008**, 20, 354012	1.8	7
100	Tuning the torsional properties of carbon nanotube systems with axial prestress. *Applied Physics Letters*, **2008**, 92, 253114	3.4	20
99	First-principles determination of static potential energy surfaces for atomic friction in MoS2 and MoO3. *Physical Review B*, **2008**, 77,	3.3	89
98	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
97	Thermal transport properties of uranium dioxide by molecular dynamics simulations. *Journal of Nuclear Materials*, **2008**, 375, 388-396	3.3	81
96	Ar beam modification of nanotube based composites using molecular dynamics simulations. *Composites Science and Technology*, **2008**, 68, 2049-2055	8.6	22
95	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
94	Computer Simulations of Nanometer-Scale Indentation and Friction **2008**, 655-740		

93	Effect of molecular interactions on carbon nanotube friction. *Journal of Applied Physics*, **2007**, 102, 064307	2.5	22
92	Ab initio molecular dynamics study of methanol adsorption on copper clusters. *Journal of Physical Chemistry A*, **2007**, 111, 441-9	2.8	25
91	Charge optimized many-body potential for the Si/SiO2 system. *Physical Review B*, **2007**, 75,	3.3	132
90	Multiscale-failure criteria of carbon nanotube systems under biaxial tension/torsion. *Nanotechnology*, **2007**, 18, 485715	3.4	11
89	Mechanistic Studies of Surface Polymerization by Ion-Assisted Deposition. *Journal of Physical Chemistry C*, **2007**, 111, 4199-4208	3.8	12
88	Investigation of the influence of thermostat configurations on the mechanical properties of carbon nanotubes in molecular dynamics simulations. *Journal of Nanoscience and Nanotechnology*, **2007**, 7, 1518-24	1.3	26
87	Prediction of high-temperature point defect formation in TiO2 from combined ab initio and thermodynamic calculations. *Acta Materialia*, **2007**, 55, 4325-4337	8.4	101
86	Combined computational and experimental study of Ar beam induced defect formation in graphite. *Nuclear Instruments & Methods in Physics Research B*, **2007**, 262, 240-248	1.2	30
85	Computational study of steric effects on the optical properties of oligomers. *Journal of Luminescence*, **2007**, 126, 278-288	3.8	3
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