Susan B Sinnott

List of Publications by Citations

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	A second-generation reactive empirical bond order (REBO) potential energy expression for hydrocarbons. *Journal of Physics Condensed Matter*, **2002**, 14, 783-802	1.8	2450
271	Model of carbon nanotube growth through chemical vapor deposition. *Chemical Physics Letters*, **1999**, 315, 25-30	2.5	460
270	Carbon Nanotubes: Synthesis, Properties, and Applications. *Critical Reviews in Solid State and Materials Sciences*, **2001**, 26, 145-249	10.1	337
269	Effect of chemical functionalization on the mechanical properties of carbon nanotubes. *Chemical Physics Letters*, **1998**, 295, 273-278	2.5	287
268	Chemical functionalization of carbon nanotubes. *Journal of Nanoscience and Nanotechnology*, **2002**, 2, 113-23	1.3	208
267	Parametrization of a reactive many-body potential for Mo□ systems. *Physical Review B*, **2009**, 79,	3.3	198
266	Topology-Scaling Identification of Layered Solids and Stable Exfoliated 2D Materials. *Physical Review Letters*, **2017**, 118, 106101	7.4	193
265	Compression of carbon nanotubes filled with C60, CH4, or Ne: predictions from molecular dynamics simulations. *Physical Review Letters*, **2002**, 88, 205505	7.4	190
264	A Computational Study of Molecular Diffusion and Dynamic Flow through Carbon Nanotubes. *Journal of Physical Chemistry B*, **2000**, 104, 4618-4624	3.4	189
263	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
262	Mechanical properties of nanotubule fibers and composites determined from theoretical calculations and simulations. *Carbon*, **1998**, 36, 1-9	10.4	166
261	Molecular dynamics simulations of the filling and decorating of carbon nanotubules. *Nanotechnology*, **1999**, 10, 273-277	3.4	156
260	Reactive Potentials for Advanced Atomistic Simulations. *Annual Review of Materials Research*, **2013**, 43, 109-129	12.8	147
259	Predicted Surface Composition and Thermodynamic Stability of MXenes in Solution. *Journal of Physical Chemistry C*, **2016**, 120, 3550-3556	3.8	143
258	Separation of Organic Molecular Mixtures in Carbon Nanotubes and Bundles: Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2001**, 105, 6916-6924	3.4	139
257	Ceramic/metal interface structures and their relationship to atomic- and meso-scale properties. *Materials Science and Engineering Reports*, **2003**, 43, 1-59	30.9	134
256	Charge optimized many-body potential for the Si□iO2 system. *Physical Review B*, **2007**, 75,	3.3	132

255	Frictional anisotropy of oriented carbon nanotube surfaces. *Tribology Letters*, **2005**, 18, 59-62	2.8	124
254	Interactions of Carbon-Nanotubule Proximal Probe Tips with Diamond and Graphene. *Physical Review Letters*, **1998**, 81, 2260-2263	7.4	123
253	Mixed Bloch-Néel-Ising character of 180° ferroelectric domain walls. *Physical Review B*, **2009**, 80,	3.3	121
252	Energetics of intrinsic point defects in uranium dioxide from electronic-structure calculations. *Journal of Nuclear Materials*, **2009**, 384, 61-69	3.3	118
251	Density functional study of the bonding in small silicon clusters. *Journal of Chemical Physics*, **1992**, 97, 4149-4161	3.9	116
250	Two-Dimensional Intrinsic Half-Metals With Large Spin Gaps. *Nano Letters*, **2017**, 17, 5251-5257	11.5	111
249	Charge-optimized many-body potential for the hafnium/hafnium oxide system. *Physical Review B*, **2010**, 81,	3.3	109
248	Behavior of molecules and molecular ions near a field emitter. *New Journal of Physics*, **2016**, 18, 033031	2.9	104
247	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
246	A Combined Computational and Experimental Study of Ion-Beam Modification of Carbon Nanotube Bundles. *Journal of Physical Chemistry B*, **2001**, 105, 12719-12725	3.4	100
245	The growth and modification of materials via ion-surface processing. *Surface Science*, **2002**, 500, 500-522	1.8	97
244	Tribological properties of carbon nanotube bundles predicted from atomistic simulations. *Surface Science*, **2001**, 487, 87-96	1.8	97
243	Stability of intrinsic defects and defect clusters in LiNbO3 from density functional theory calculations. *Physical Review B*, **2008**, 78,	3.3	96
242	Molecular Dynamics Simulation Study of Carbon Nanotube Welding under Electron Beam Irradiation. *Nano Letters*, **2004**, 4, 109-114	11.5	96
241	Ion separation using a Y-junction carbon nanotube. *Nanotechnology*, **2006**, 17, 895-900	3.4	91
240	First-principles determination of static potential energy surfaces for atomic friction in MoS2 and MoO3. *Physical Review B*, **2008**, 77,	3.3	89
239	Corrected effective-medium study of metal-surface relaxation. *Physical Review B*, **1991**, 44, 8927-8941	3.3	84
238	A reactive empirical bond order (REBO) potential for hydrocarbon-oxygen interactions. *Journal of Physics Condensed Matter*, **2004**, 16, 7261-7275	1.8	83

237	Thermal transport properties of uranium dioxide by molecular dynamics simulations. *Journal of Nuclear Materials*, **2008**, 375, 388-396	3.3	81
236	Second-generation charge-optimized many-body potential for Si/SiO2 and amorphous silica. *Physical Review B*, **2010**, 82,	3.3	79
235	Sorption of Butane on Carbon Multiwall Nanotubes at Room Temperature. *Langmuir*, **2001**, 17, 7540-7544	4	78
234	Variable charge reactive potential for hydrocarbons to simulate organic-copper interactions. *Journal of Physical Chemistry A*, **2012**, 116, 7976-91	2.8	76
233	Effect of polyatomic ion structure on thin-film growth: Experiments and molecular dynamics simulations. *Journal of Applied Physics*, **2000**, 88, 5004-5016	2.5	75
232	Chemical functionalization of carbon nanotubes through energetic radical collisions. *Physical Review B*, **2000**, 61, R16343-R16346	3.3	74
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	Carbon doping of WS monolayers: Bandgap reduction and p-type doping transport. *Science Advances*, **2019**, 5, eaav5003	14.3	70
229	Tensile mechanical behavior of hollow and filled carbon nanotubes under tension or combined tension-torsion. *Applied Physics Letters*, **2007**, 90, 023102	3.4	70
228	Elastic torsional responses of carbon nanotube systems. *Journal of Applied Physics*, **2007**, 101, 084309	2.5	70
227	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
226	Computational characterization of lightweight multilayer MXene Li-ion battery anodes. *Applied Physics Letters*, **2016**, 108, 023901	3.4	66
225	Friction Properties of Carbon Nano-Onions from Experiment and Computer Simulations. *Tribology Letters*, **2010**, 37, 75-81	2.8	64
224	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
223	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
222	Atomistic simulations of copper oxidation and Cu/Cu2O interfaces using charge-optimized many-body potentials. *Physical Review B*, **2011**, 84,	3.3	59
221	Transition from thermal to athermal friction under cryogenic conditions. *Physical Review Letters*, **2009**, 102, 186102	7.4	58
220	Effects of unique ion chemistry on thin-film growth by plasma-surface interactions. *Proceedings of the National Academy of Sciences of the United States of America*, **2000**, 97, 23-7	11.5	56

219	Computational discovery of stable M2AX phases. *Physical Review B*, **2016**, 94,	3.3	50
218	Multiscale computational understanding and growth of 2D materials: a review. *Npj Computational Materials*, **2020**, 6,	10.9	49
217	Predictions of a spiral diffusion path for nonspherical organic molecules in carbon nanotubes. *Physical Review Letters*, **2002**, 89, 278301	7.4	49
216	Variable charge many-body interatomic potentials. *MRS Bulletin*, **2012**, 37, 504-512	3.2	48
215	Thermal Transport in Off-Stoichiometric Uranium Dioxide by Atomic Level Simulation. *Journal of the American Ceramic Society*, **2009**, 92, 850-856	3.8	47
214	Molecular dynamics simulations of electron and ion beam irradiation of multiwalled carbon nanotubes: The effects on failure by inner tube sliding. *Physical Review B*, **2006**, 73,	3.3	47
213	Critical assessment of UO2 classical potentials for thermal conductivity calculations. *Journal of Materials Science*, **2012**, 47, 7693-7702	4.3	46
212	Segregation of xenon to dislocations and grain boundaries in uranium dioxide. *Physical Review B*, **2011**, 84,	3.3	46
211	Thermodynamics of fission products in UO(2 − x). *Journal of Physics Condensed Matter*, **2009**, 21, 435602	1.8	45
210	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
209	Sliding orientation effects on the tribological properties of polytetrafluoroethylene. *Journal of Applied Physics*, **2007**, 102, 123509	2.5	43
208	Molecular dynamics study of the adhesion of Cu/SiO2 interfaces using a variable-charge interatomic potential. *Physical Review B*, **2011**, 83,	3.3	42
207	Energetics of Oxidation in MoS2 Nanoparticles by Density Functional Theory. *Journal of Physical Chemistry C*, **2011**, 115, 10606-10616	3.8	42
206	Atomistic simulations of the nanometer-scale indentation of amorphous-carbon thin films. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **1997**, 15, 936-940	2.9	42
205	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
204	Computational discovery and characterization of polymorphic two-dimensional IVV materials. *Applied Physics Letters*, **2016**, 109, 192103	3.4	41
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202	Fitting empirical potentials: Challenges and methodologies. *Current Opinion in Solid State and Materials Science*, **2013**, 17, 263-270	12	39

201	Three decades of many-body potentials in materials research. *MRS Bulletin*, **2012**, 37, 469-473	3.2	39
200	A critical assessment of interatomic potentials for ceria with application to its elastic properties. *Solid State Ionics*, **2010**, 181, 551-556	3.3	39
199	Effects of edge dislocations on thermal transport in UO2. *Journal of Nuclear Materials*, **2013**, 434, 203-209	3.3	38
198	Lubrication mechanisms of hollow-core inorganic fullerene-like nanoparticles: coupling experimental and computational works. *Nanotechnology*, **2012**, 23, 375701	3.4	38
197	Stability and charge transfer levels of extrinsic defects in LiNbO3. *Physical Review B*, **2010**, 82,	3.3	38
196	Molecular dynamics of carbon nanotubule proximal probe tip-surface contacts. *Physical Review B*, **1999**, 60, 13786-13791	3.3	38
195	Structure and energetics of 180° domain walls in PbTiO3 by density functional theory. *Journal of Physics Condensed Matter*, **2011**, 23, 175902	1.8	37
194	Modification of carbon nanotube-polystyrene matrix composites through polyatomic-ion beam deposition predictions from molecular dynamics simulations. *Composites Science and Technology*, **2003**, 63, 1663-1669	8.6	37
193	Mechanical behavior of MoS2 nanotubes under compression, tension, and torsion from molecular dynamics simulations. *Journal of Applied Physics*, **2012**, 112, 123510	2.5	36
192	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
191	Torsional stiffening of carbon nanotube systems. *Applied Physics Letters*, **2007**, 91, 093102	3.4	36
190	Equilibrium and nonequilibrium transport of oxygen in carbon nanotubes. *Nano Letters*, **2005**, 5, 793-8	11.5	36
189	Predicted mechanical properties of a coiled carbon nanotube. *Carbon*, **2012**, 50, 968-976	10.4	35
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187	Surface patterning by atomically-controlled chemical forces: molecular dynamics simulations. *Surface Science*, **1994**, 316, L1055-L1060	1.8	34
186	Molecular dynamics investigation of the lubrication mechanism of carbon nano-onions. *Computational Materials Science*, **2012**, 54, 91-96	3.2	33
185	Structure and energetics of Er defects in LiNbO3 from first-principles and thermodynamic calculations. *Physical Review B*, **2009**, 80,	3.3	33
184	Ab Initio Calculations of Pristine and Doped Zirconia Σ5 (310)/[001] Tilt Grain Boundaries. *Journal of the American Ceramic Society*, **2002**, 85, 1594-1600	3.8	33

183	Materials science. Simulating multifunctional structures. *Science*, **2009**, 325, 1634-5	33.3	32
182	Simulated engineering of nanostructures. *Nanotechnology*, **1996**, 7, 161-167	3.4	32
181	Computational Studies of Non-Equilibrium Molecular Transport through Carbon Nanotubes. *Journal of Physical Chemistry B*, **2004**, 108, 9861-9870	3.4	32
180	Molecular Dynamics Simulations of the Chemical Modification of Polystyrene through CxFy+ Beam Deposition. *Journal of Physical Chemistry B*, **2004**, 108, 18993-19001	3.4	32
179	Polymerization via Cluster□Solid Surface Impacts: Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **1997**, 101, 6883-6890	3.4	31
178	Structure and diffusion of intrinsic defect complexes in LiNbO□from density functional theory calculations. *Journal of Physics Condensed Matter*, **2010**, 22, 135002	1.8	30
177	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
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175	Ab Initio Calculations of Intrinsic Defects in Rutile TiO2. *Journal of the American Ceramic Society*, **2005**, 88, 737-741	3.8	30
174	Stoichiometry of the LaFeO3 (010) surface determined from first-principles and thermodynamic calculations. *Physical Review B*, **2011**, 83,	3.3	29
173	Reparameterization of the REBO-CHO potential for graphene oxide molecular dynamics simulations. *Physical Review B*, **2011**, 84,	3.3	29
172	Energetics of charged point defects in rutile TiO2 by density functional theory. *Acta Materialia*, **2009**, 57, 5882-5891	8.4	29
171	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
170	Molecular dynamics simulations of polyatomic-ion beam deposition-induced chemical modification of carbon nanotube/polymer composites. *Journal of Materials Chemistry*, **2004**, 14, 719		29
169	Comparison of morphology and mechanical properties of surfactant aggregates at water-silica and water-graphite interfaces from molecular dynamics simulations. *Journal of Colloid and Interface Science*, **2006**, 296, 342-9	9.3	28
168	Nanostructure of Fluorocarbon Films Deposited on Polystyrene from Hyperthermal C3F5+ Ions. *Journal of Physical Chemistry B*, **2004**, 108, 9656-9664	3.4	28
167	Graphene-Titanium Interfaces from Molecular Dynamics Simulations. *ACS Applied Materials & Interfaces*, **2017**, 9, 33288-33297	9.5	27
166	Atomic-Level Simulation of Ferroelectricity in Oxides: Current Status and Opportunities. *Annual Review of Materials Research*, **2007**, 37, 239-270	12.8	27

165	Effect of filling on the compressibility of carbon nanotubes: predictions from molecular dynamics simulations. *Journal of Nanoscience and Nanotechnology*, **2005**, 5, 536-41	1.3	27
164	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
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161	The effect of normal load on polytetrafluoroethylene tribology. *Journal of Physics Condensed Matter*, **2009**, 21, 144201	1.8	25
160	Ab initio molecular dynamics study of methanol adsorption on copper clusters. *Journal of Physical Chemistry A*, **2007**, 111, 441-9	2.8	25
159	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
158	Effect of Temperature on the Friction and Wear of PTFE by Atomic-Level Simulation. *Tribology Letters*, **2015**, 58, 1	2.8	23
157	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
156	Data-Driven Model for Estimation of Friction Coefficient Via Informatics Methods. *Tribology Letters*, **2012**, 47, 211-221	2.8	23
155	Ab initio calculations of rigid-body displacements at the Σ5 (210) tilt grain boundary in TiO2. *Physical Review B*, **2000**, 61, 15645-15648	3.3	23
154	Nanoindentation of Zr by molecular dynamics simulation. *Journal of Nuclear Materials*, **2015**, 467, 742-757	3.3	22
153	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
152	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
151	Effect of molecular interactions on carbon nanotube friction. *Journal of Applied Physics*, **2007**, 102, 064307	2.5	22
150	Ar beam modification of nanotube based composites using molecular dynamics simulations. *Composites Science and Technology*, **2008**, 68, 2049-2055	8.6	22
149	Deformation processes in polycrystalline Zr by molecular dynamics simulations. *Journal of Nuclear Materials*, **2015**, 462, 147-159	3.3	21
148	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

147	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
146	Properties of Ti/TiC Interfaces from Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2016**, 120, 12530-12538	3.8	21
145	A charge optimized many-body (COMB) potential for titanium and titania. *Journal of Physics Condensed Matter*, **2014**, 26, 315007	1.8	20
144	Charge-optimized many-body (COMB) potential for zirconium. *Journal of Nuclear Materials*, **2013**, 441, 274-279	3.3	20
143	Mapping Chemical Selection Pathways for Designing Multicomponent Alloys: an informatics framework for materials design. *Scientific Reports*, **2015**, 5, 17960	4.9	20
142	Influence of the Molecular Level Structure of Polyethylene and Polytetrafluoroethylene on Their Tribological Response. *Tribology Letters*, **2011**, 42, 193-201	2.8	20
141	Intrinsic electrostatic effects in nanostructured ceramics. *Physical Review B*, **2010**, 81,	3.3	20
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139	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
138	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
137	Computational and experimental studies of phase separation in pentacene:C60 mixtures. *Journal of Vacuum Science & Technology B*, **2009**, 27, 169		19
136	Effect of ionic polarizability on oxygen diffusion in Bi2O3 from atomistic simulation. *Ionics*, **2010**, 16, 297-303	2.7	19
135	Preferred crystallographic orientation relationships of nickel films deposited on (100) cubic-zirconia substrates. *Thin Solid Films*, **2000**, 372, 37-44	2.2	19
134	Primary radiation defect production in polyethylene and cellulose. *Journal of Physical Chemistry B*, **2012**, 116, 13932-8	3.4	18
133	Piecewise-stationary bandit problems with side observations **2009**,		18
132	Predicting the Electrochemical Synthesis of 2D Materials from First Principles. *Journal of Physical Chemistry C*, **2019**, 123, 3180-3187	3.8	18
131	Three-dimensional atomic scale electron density reconstruction of octahedral tilt epitaxy in functional perovskites. *Nature Communications*, **2018**, 9, 5220	17.4	18
130	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

129	Generation of 3D hydrocarbon thin films via organic molecular cluster collisions. *Surface Science*, **1998**, 398, 195-202	1.8	17
128	Cu cluster deposition on ZnO10$\bar{1}$0: Morphology and growth mode predicted from molecular dynamics simulations. *Surface Science*, **2014**, 621, 109-116	1.8	16
127	Unique buckling responses of multi-walled carbon nanotubes incorporated as torsion springs. *Carbon*, **2010**, 48, 1697-1701	10.4	16
126	Nanoindentation of ZrO2 and ZrO2/Zr systems by molecular dynamics simulation. *Journal of Nuclear Materials*, **2017**, 486, 250-266	3.3	15
125	Molecular Simulation of Capture of Sulfur-Containing Gases by Porous Aromatic Frameworks. *Journal of Physical Chemistry C*, **2018**, 122, 18456-18467	3.8	15
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119	Charge Optimized Many Body (COMB) potentials for simulation of nuclear fuel and clad. *Computational Materials Science*, **2018**, 148, 231-241	3.2	14
118	Classical interatomic potential for orthorhombic uranium. *Journal of Physics Condensed Matter*, **2012**, 24, 235403	1.8	14
117	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
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115	Interaction of functionalized benzene molecules with carbon nanopores. *Chemical Physics Letters*, **2004**, 389, 96-100	2.5	14
114	Anisotropy in oxidation of zirconium surfaces from density functional theory calculations. *Computational Materials Science*, **2015**, 98, 112-116	3.2	13
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108	Effect of Surface Chemistry on Water Interaction with Cu(111). *Langmuir*, **2016**, 32, 8061-70	4	13
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106	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
105	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
104	Effect of cluster size on the reactivity of organic molecular clusters: Atomistic simulations. *Nuclear Instruments & Methods in Physics Research B*, **1998**, 140, 39-46	1.2	12
103	Mechanistic Studies of Surface Polymerization by Ion-Assisted Deposition. *Journal of Physical Chemistry C*, **2007**, 111, 4199-4208	3.8	12
102	Computational Investigation of the Chemical Modification of Polystyrene through Fluorocarbon and Hydrocarbon Ion Beam Deposition. *Chemistry of Materials*, **2006**, 18, 914-921	9.6	12
101	A molecular dynamics study of thin-film formation via molecular cluster beam deposition: effect of incident species. *Surface Science*, **2003**, 526, 230-242	1.8	12
100	Adhesion and diffusion at TiN/TiO2 interfaces: A first principles study. *Computational Materials Science*, **2017**, 130, 249-256	3.2	11
99	On the Multiple Event Detection in Atom Probe Tomography. *Microscopy and Microanalysis*, **2017**, 23, 618-619	0.5	11
98	Applied Potentials in Variable-Charge Reactive Force Fields for Electrochemical Systems. *Journal of Physical Chemistry A*, **2018**, 122, 631-638	2.8	11
97	Potential Optimization Software for Materials (POSMat). *Computer Physics Communications*, **2016**, 203, 201-211	4.2	11
96	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
95	Morphology and growth modes of metal-oxides deposited on SrTiO3. *Surface Science*, **2009**, 603, 873-880	1.8	11
94	Coupling of surface relaxation and polarization in PbTiO3from atomistic simulation. *Journal of Physics Condensed Matter*, **2008**, 20, 395004	1.8	11

93	Multiscale-failure criteria of carbon nanotube systems under biaxial tension–torsion. *Nanotechnology*, **2007**, 18, 485715	3.4	11
92	Thin-film nucleation through molecular cluster beam deposition: Comparison of tight-binding and many-body empirical potential molecular dynamics simulations. *Journal of Chemical Physics*, **2002**, 116, 6738-6744	3.9	11
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90	Dependence of plasma-induced modification of polymer surfaces on polyatomic ion chemistry. *Applied Physics Letters*, **2004**, 84, 5118-5120	3.4	10
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