Bobby G Sumpter

List of Publications by Year
in descending order

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535 papers	27,017 citations	7551 77 h-index	9553 142 g-index
554 all docs	554 docs citations	554 times ranked	31997 citing authors

#	Article	IF	Citations
1	Recent Advances in Two-Dimensional Materials beyond Graphene. ACS Nano, 2015, 9, 11509-11539.	7.3	2,069
2	Ultrathin Planar Graphene Supercapacitors. Nano Letters, 2011, 11, 1423-1427.	4.5	1,145
3	Controlled Formation of Sharp Zigzag and Armchair Edges in Graphitic Nanoribbons. Science, 2009, 323, 1701-1705.	6.0	655
4	Density-functional approaches to noncovalent interactions: A comparison of dispersion corrections (DFT-D), exchange-hole dipole moment (XDM) theory, and specialized functionals. Journal of Chemical Physics, 2011, 134, 084107.	1.2	607
5	A Universal Model for Nanoporous Carbon Supercapacitors Applicable to Diverse Pore Regimes, Carbon Materials, and Electrolytes. Chemistry - A European Journal, 2008, 14, 6614-6626.	1.7	545
6	Theoretical Model for Nanoporous Carbon Supercapacitors. Angewandte Chemie - International Edition, 2008, 47, 520-524.	7.2	526
7	PdSe₂: Pentagonal Two-Dimensional Layers with High Air Stability for Electronics. Journal of the American Chemical Society, 2017, 139, 14090-14097.	6.6	509
8	Electronic Bandgap and Edge Reconstruction in Phosphorene Materials. Nano Letters, 2014, 14, 6400-6406.	4.5	459
9	Unique chemical reactivity of a graphene nanoribbonâ€™s zigzag edge. Journal of Chemical Physics, 2007, 126, 134701.	1.2	423
10	Covalently bonded three-dimensional carbon nanotube solids via boron induced nanojunctions. Scientific Reports, 2012, 2, 363.	1.6	329
11	Anisotropic Electron-Photon and Electron-Phonon Interactions in Black Phosphorus. Nano Letters, 2016, 16, 2260-2267.	4.5	328
12	Bigâ€“deepâ€“smart data in imaging for guiding materials design. Nature Materials, 2015, 14, 973-980.	13.3	281
13	A physical catalyst for the electrolysis of nitrogen to ammonia. Science Advances, 2018, 4, e1700336.	4.7	264
14	Highâ€Selectivity Electrochemical Conversion of CO₂ to Ethanol using a Copper Nanoparticle/Nâ€Doped Graphene Electrode. ChemistrySelect, 2016, 1, 6055-6061.	0.7	251
15	Ultrathin nanosheets of CrSiTe₃: a semiconducting two-dimensional ferromagnetic material. Journal of Materials Chemistry C, 2016, 4, 315-322.	2.7	235
16	Electronic Transport and Mechanical Properties of Phosphorus- and Phosphorusâ^'Nitrogen-Doped Carbon Nanotubes. ACS Nano, 2009, 3, 1913-1921.	7.3	228
17	Transitionâ€Metal Substitution Doping in Synthetic Atomically Thin Semiconductors. Advanced Materials, 2016, 28, 9735-9743.	11.1	208
18	Nitrogen-Mediated Carbon Nanotube Growth: Diameter Reduction, Metallicity, Bundle Dispersability, and Bamboo-like Structure Formation. ACS Nano, 2007, 1, 369-375.	7.3	207

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19	Tunable water desalination across graphene oxide framework membranes. Physical Chemistry Chemical Physics, 2014, 16, 8646.	1.3	194
20	Heterodoped Nanotubes: Theory, Synthesis, and Characterization of Phosphorusâ^'Nitrogen Doped Multiwalled Carbon Nanotubes. ACS Nano, 2008, 2, 441-448.	7.3	192
21	How Do Aryl Groups Attach to a Graphene Sheet?. Journal of Physical Chemistry B, 2006, 110, 23628-23632.	1.2	191
22	First principles study of magnetism in nanographenes. Journal of Chemical Physics, 2007, 127, 124703.	1.2	191
23	Complex Capacitance Scaling in Ionic Liquids-Filled Nanopores. ACS Nano, 2011, 5, 9044-9051.	7.3	188
24	Ion Distribution in Electrified Micropores and Its Role in the Anomalous Enhancement of Capacitance. ACS Nano, 2010, 4, 2382-2390.	7.3	183
25	Chemical nature of ferroelastic twin domains in CH3NH3PbI3 perovskite. Nature Materials, 2018, 17, 1013-1019.	13.3	183
26	Low-Frequency Interlayer Breathing Modes in Few-Layer Black Phosphorus. Nano Letters, 2015, 15, 4080-4088.	4.5	182
27	The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design. Npj Computational Materials, 2020, 6, .	3.5	181
28	Low-Frequency Shear and Layer-Breathing Modes in Raman Scattering of Two-Dimensional Materials. ACS Nano, 2017, 11, 11777-11802.	7.3	179
29	Low-Frequency Interlayer Raman Modes to Probe Interface of Twisted Bilayer MoS₂. Nano Letters, 2016, 16, 1435-1444.	4.5	177
30	Big Effect of Small Nanoparticles: A Shift in Paradigm for Polymer Nanocomposites. ACS Nano, 2017, 11, 752-759.	7.3	177
31	Dynamics of fluid flow inside carbon nanotubes. Nanotechnology, 1996, 7, 241-246.	1.3	176
32	The importance of ion size and electrode curvature on electrical double layers in ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 1152-1161.	1.3	173
33	Controlling Interfacial Dynamics: Covalent Bonding versus Physical Adsorption in Polymer Nanocomposites. ACS Nano, 2016, 10, 6843-6852.	7.3	152
34	Low-Frequency Raman Fingerprints of Two-Dimensional Metal Dichalcogenide Layer Stacking Configurations. ACS Nano, 2015, 9, 6333-6342.	7.3	151
35	Symplectic integrators for large scale molecular dynamics simulations: A comparison of several explicit methods. Journal of Chemical Physics, 1994, 101, 4062-4072.	1.2	149
36	Electronic structure and properties of isoreticular metal-organic frameworks: The case of M-IRMOF1 (M=Zn, Cd, Be, Mg, and Ca). Journal of Chemical Physics, 2005, 123, 124713.	1.2	147

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37	Curvature effects in carbon nanomaterials: Exohedral versus endohedral supercapacitors. Journal of Materials Research, 2010, 25, 1525-1531.	1.2	142
38	Synthesis, Electronic Structure, and Raman Scattering of Phosphorus-Doped Single-Wall Carbon Nanotubes. Nano Letters, 2009, 9, 2267-2272.	4.5	134
39	Understanding the origin of high-rate intercalation pseudocapacitance in Nb2O5 crystals. Journal of Materials Chemistry A, 2013, 1, 14951.	5.2	134
40	Structure and Bonding between an Aryl Group and Metal Surfaces. Journal of the American Chemical Society, 2006, 128, 6030-6031.	6.6	131
41	Surface-Induced Orientation Control of CuPc Molecules for the Epitaxial Growth of Highly Ordered Organic Crystals on Graphene. Journal of the American Chemical Society, 2013, 135, 3680-3687.	6.6	125
42	Structural, magnetic, and transport properties of substitutionally doped graphene nanoribbons from first principles. Physical Review B, 2011, 83, .	1.1	124
43	High-Performance Field-Effect Transistors Based on Polystyrene-b-Poly(3-hexylthiophene) Diblock Copolymers. ACS Nano, 2011, 5, 3559-3567.	7.3	122
44	Enhanced Raman Scattering on In-Plane Anisotropic Layered Materials. Journal of the American Chemical Society, 2015, 137, 15511-15517.	6.6	122
45	Tailoring Vacancies Far Beyond Intrinsic Levels Changes the Carrier Type and Optical Response in Monolayer MoSe_{2â"x} Crystals. Nano Letters, 2016, 16, 5213-5220.	4.5	121
46	Boron Nitride Nanoribbons Become Metallic. Nano Letters, 2011, 11, 3267-3273.	4.5	120
47	Nanoscale Ferroelectricity in Crystalline Î³â€Glycine. Advanced Functional Materials, 2012, 22, 2996-3003.	7.8	119
48	Step-by-step growth of epitaxially aligned polythiophene by surface-confined reaction. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 11200-11204.	3.3	117
49	Twisted MoSe₂ Bilayers with Variable Local Stacking and Interlayer Coupling Revealed by Low-Frequency Raman Spectroscopy. ACS Nano, 2016, 10, 2736-2744.	7.3	117
50	In-Plane Heterojunctions Enable Multiphasic Two-Dimensional (2D) MoS₂ Nanosheets As Efficient Photocatalysts for Hydrogen Evolution from Water Reduction. ACS Catalysis, 2016, 6, 6723-6729.	5.5	116
51	Interfacial Properties of Polymer Nanocomposites: Role of Chain Rigidity and Dynamic Heterogeneity Length Scale. Macromolecules, 2017, 50, 2397-2406.	2.2	115
52	Focus: Structure and dynamics of the interfacial layer in polymer nanocomposites with attractive interactions. Journal of Chemical Physics, 2017, 146, 203201.	1.2	114
53	Deep learning analysis of defect and phase evolution during electron beam-induced transformations in WS2. Npj Computational Materials, 2019, 5, .	3.5	113
54	Benchmarking graph neural networks for materials chemistry. Npj Computational Materials, 2021, 7, .	3.5	113

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55	Theory and Applications of Neural Computing in Chemical Science. Annual Review of Physical Chemistry, 1994, 45, 439-481.	4.8	111
56	Heterojunctions between metals and carbon nanotubes as ultimate nanocontacts. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 4591-4595.	3.3	110
57	PSâ€bâ€P3HT Copolymers as P3HT/PCBM Interfacial Compatibilizers for High Efficiency Photovoltaics. Advanced Materials, 2011, 23, 5529-5535.	11.1	110
58	Untangling the Effects of Chain Rigidity on the Structure and Dynamics of Strongly Adsorbed Polymer Melts. Macromolecules, 2015, 48, 4207-4219.	2.2	109
59	Machine learned features from density of states for accurate adsorption energy prediction. Nature Communications, 2021, 12, 88.	5.8	108
60	Structure and dynamics of electrical double layers in organic electrolytes. Physical Chemistry Chemical Physics, 2010, 12, 5468.	1.3	107
61	The isotopic effects of deuteration on optoelectronic properties of conducting polymers. Nature Communications, 2014, 5, 3180.	5.8	103
62	Van der Waals Epitaxial Growth of Two-Dimensional Single-Crystalline GaSe Domains on Graphene. ACS Nano, 2015, 9, 8078-8088.	7.3	103
63	Phosphorus and phosphorusâ€“nitrogen doped carbon nanotubes for ultrasensitive and selective molecular detection. Nanoscale, 2011, 3, 1008-1013.	2.8	102
64	Ultrafast Charge Transfer and Hybrid Exciton Formation in 2D/0D Heterostructures. Journal of the American Chemical Society, 2016, 138, 14713-14719.	6.6	102
65	Directing Matter: Toward Atomic-Scale 3D Nanofabrication. ACS Nano, 2016, 10, 5600-5618.	7.3	99
66	Oxidative Dehydrogenation of Propane to Propylene with Soft Oxidants via Heterogeneous Catalysis. ACS Catalysis, 2021, 11, 2182-2234.	5.5	97
67	Computer experiments on the internal dynamics of crystalline polyethylene: Mechanistic details of conformational disorder. Journal of Chemical Physics, 1990, 93, 6875-6889.	1.2	95
68	Morphologies of block copolymers composed of charged and neutral blocks. Soft Matter, 2012, 8, 3036.	1.2	95
69	Assessment of standard force field models against highâ€qualityab initiopotential curves for prototypes of Ï€â€“Ï€, CH/Ï€, and SH/Ï€ interactions. Journal of Computational Chemistry, 2009, 30, 2187-2193.	1.5	93
70	An Assessment of Density Functional Methods for Potential Energy Curves of Nonbonded Interactions: The XYG3 and B97-D Approximations. Journal of Chemical Theory and Computation, 2010, 6, 727-734.	2.3	91
71	A â€œcounter-charge layer in generalized solventsâ€•framework for electrical double layers in neat and hybrid ionic liquid electrolytes. Physical Chemistry Chemical Physics, 2011, 13, 14723.	1.3	90
72	Continuum methods of mechanics as a simplified approach to structural engineering of nanostructures. Nanotechnology, 1998, 9, 30-36.	1.3	87

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73	Dynamics of a laser driven molecular motor. Nanotechnology, 1995, 6, 52-63.	1.3	84
74	Radical Chemistry and Reaction Mechanisms of Propane Oxidative Dehydrogenation over Hexagonal Boron Nitride Catalysts. Angewandte Chemie - International Edition, 2020, 59, 8042-8046.	7.2	83
75	Nanoforging Single Layer MoSe2 Through Defect Engineering with Focused Helium Ion Beams. Scientific Reports, 2016, 6, 30481.	1.6	82
76	Influence of Chain Rigidity and Dielectric Constant on the Glass Transition Temperature in Polymerized Ionic Liquids. Journal of Physical Chemistry B, 2017, 121, 11511-11519.	1.2	82
77	Atomistic dynamics of macromolecular crystals. , 1994, , 27-72.		81
78	The dynamics of molecular bearings. Nanotechnology, 1995, 6, 64-74.	1.3	81
79	Alloy Engineering of Defect Properties in Semiconductors: Suppression of Deep Levels in Transition-Metal Dichalcogenides. Physical Review Letters, 2015, 115, 126806.	2.9	81
80	Potential energy surfaces for macromolecules. A neural network technique. Chemical Physics Letters, 1992, 192, 455-462.	1.2	78
81	Importance of Ion Packing on the Dynamics of Ionic Liquids during Micropore Charging. Journal of Physical Chemistry Letters, 2016, 7, 36-42.	2.1	78
82	Computational Study of the Structure, Dynamics, and Photophysical Properties of Conjugated Polymers and Oligomers under Nanoscale Confinement. Journal of Physical Chemistry B, 2005, 109, 7671-7685.	1.2	77
83	Voltage Dependent Charge Storage Modes and Capacity in Subnanometer Pores. Journal of Physical Chemistry Letters, 2012, 3, 1732-1737.	2.1	77
84	Neural Network-Graph Theory Approach to the Prediction of the Physical Properties of Organic Compounds. Journal of Chemical Information and Computer Sciences, 1994, 34, 832-839.	2.8	76
85	An Atomistic Branching Mechanism for Carbon Nanotubes: Sulfur as the Triggering Agent. Angewandte Chemie - International Edition, 2008, 47, 2948-2953.	7.2	76
86	Enhancing Ion Migration in Grain Boundaries of Hybrid Organicâ€“Inorganic Perovskites by Chlorine. Advanced Functional Materials, 2017, 27, 1700749.	7.8	74
87	Prediction of Carbon Dioxide Adsorption via Deep Learning. Angewandte Chemie - International Edition, 2019, 58, 259-263.	7.2	74
88	Atomicâ€Łevel Sculpting of Crystalline Oxides: Toward Bulk Nanofabrication with Single Atomic Plane Precision. Small, 2015, 11, 5895-5900.	5.2	73
89	Density Functional Studies of Stoichiometric Surfaces of Orthorhombic Hybrid Perovskite CH₃NH₃PbI₃. Journal of Physical Chemistry C, 2015, 119, 1136-1145.	1.5	73
90	Strain-engineered optoelectronic properties of 2D transition metal dichalcogenide lateral heterostructures. 2D Materials, 2017, 4, 021016.	2.0	72

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91	Molecular dynamics simulations of polymers: Methods for optimal Fortran programming. Journal of Computational Chemistry, 1990, 11, 236-241.	1.5	71
92	Quantum Transport in Graphene Nanonetworks. Nano Letters, 2011, 11, 3058-3064.	4.5	71
93	Spatially resolved one-dimensional boundary states in grapheneâ€“hexagonal boron nitride planar heterostructures. Nature Communications, 2014, 5, 5403.	5.8	71
94	A theoretical and experimental study on manipulating the structure and properties of carbon nanotubes using substitutional dopants. International Journal of Quantum Chemistry, 2009, 109, 97-118.	1.0	70
95	Building and exploring libraries of atomic defects in graphene: Scanning transmission electron and scanning tunneling microscopy study. Science Advances, 2019, 5, eaaw8989.	4.7	70
96	On the Design, Analysis, and Characterization of Materials Using Computational Neural Networks. Annual Review of Materials Research, 1996, 26, 223-277.	5.5	67
97	Duality of the interfacial thermal conductance in graphene-based nanocomposites. Carbon, 2014, 75, 169-177.	5.4	67
98	Aminopolymer functionalization of boron nitride nanosheets for highly efficient capture of carbon dioxide. Journal of Materials Chemistry A, 2017, 5, 16241-16248.	5.2	67
99	3D Imaging and Manipulation of Subsurface Selenium Vacancies in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>PdSe</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn> Physical Review Letters, 2018, 121, 086101.	2.9	66
100	Structure and Stability of Small Boron and Boron Oxide Clusters. Journal of Physical Chemistry A, 2007, 111, 6539-6551.	1.1	65
101	A comparative study of phosphoric acidâ€doped mâ€PBI membranes. Journal of Polymer Science, Part B: Polymer Physics, 2014, 52, 26-35.	2.4	65
102	Size-Expanded DNA Bases:Â An Ab Initio Study of Their Structural and Electronic Properties. Journal of Physical Chemistry B, 2005, 109, 21135-21139.	1.2	64
103	Thermodynamics and Kinetics of Gas Storage in Porous Liquids. Journal of Physical Chemistry B, 2016, 120, 7195-7200.	1.2	64
104	Supramolecular Self-Assembly of Ï€-Conjugated Hydrocarbons via 2D Cooperative CH/Ï€ Interaction. ACS Nano, 2012, 6, 566-572.	7.3	63
105	Amphoteric doping of carbon nanotubes by encapsulation of organic molecules: Electronic properties and quantum conductance. Journal of Chemical Physics, 2005, 123, 024705.	1.2	62
106	Molecular dynamics simulation of the condis state of polyethylene. Macromolecules, 1990, 23, 664-669.	2.2	61
107	UV-activated ZnO films on a flexible substrate for room temperature O2 and H2O sensing. Scientific Reports, 2017, 7, 6053.	1.6	61
108	Spin Polarized Conductance in Hybrid Graphene Nanoribbons Using 5â”7 Defects. ACS Nano, 2009, 3, 3606-3612.	7.3	60

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109	Anomalous interlayer vibrations in strongly coupled layered PdSe ₂. 2D Materials, 2018, 5, 035016.	2.0	60
110	Solvent-type-dependent polymorphism and charge transport in a long fused-ring organic semiconductor. Nanoscale, 2014, 6, 449-456.	2.8	59
111	Highly stable two-dimensional silicon phosphides: Different stoichiometries and exotic electronic properties. Physical Review B, 2015, 91, .	1.1	58
112	PEDOT:PSS/QCM-based multimodal humidity and pressure sensor. Sensors and Actuators B: Chemical, 2016, 236, 91-98.	4.0	58
113	Controllable conversion of quasi-freestanding polymer chains to graphene nanoribbons. Nature Communications, 2017, 8, 14815.	5.8	58
114	Dynamics of flow inside carbon nanotubes. Nanotechnology, 1997, 8, 112-118.	1.3	57
115	Revealing spatially heterogeneous relaxation in a model nanocomposite. Journal of Chemical Physics, 2015, 143, 194704.	1.2	57
116	Engineering the Bacterial Microcompartment Domain for Molecular Scaffolding Applications. Frontiers in Microbiology, 2017, 8, 1441.	1.5	57
117	Photon Antibunching from Oriented Semiconducting Polymer Nanostructures. Journal of the American Chemical Society, 2004, 126, 3376-3377.	6.6	56
118	Controlling Edge Morphology in Graphene Layers Using Electron Irradiation: From Sharp Atomic Edges to Coalesced Layers Forming Loops. Physical Review Letters, 2010, 105, 045501.	2.9	56
119	Amphiphilic Bottlebrush Block Copolymers: Analysis of Aqueous Self-Assembly by Small-Angle Neutron Scattering and Surface Tension Measurements. Macromolecules, 2019, 52, 465-476.	2.2	56
120	Computational neural networks and the rational design of polymeric materials: the next generation polycarbonates. Computational and Theoretical Polymer Science, 1998, 8, 311-321.	1.1	55
121	Theoretical Study on the Structure, Stability, and Electronic Properties of the Guanineâ^'Znâ^'Cytosine Base Pair in M-DNA. Journal of Physical Chemistry B, 2007, 111, 870-879.	1.2	55
122	Comparison of classical and quantum phase space structure of nonrigid molecules, LiCN. Chemical Physics Letters, 1989, 161, 60-66.	1.2	54
123	Clean Nanotube Unzipping by Abrupt Thermal Expansion of Molecular Nitrogen: Graphene Nanoribbons with Atomically Smooth Edges. ACS Nano, 2012, 6, 2261-2272.	7.3	54
124	Novel methods for spectral analysis. Physics Reports, 1991, 205, 109-152.	10.3	53
125	Effect of diffuse layer and pore shapes in mesoporous carbon supercapacitors. Journal of Materials Research, 2010, 25, 1469-1475.	1.2	53
126	Atomistic Insight on the Charging Energetics in Subnanometer Pore Supercapacitors. Journal of Physical Chemistry C, 2010, 114, 18012-18016.	1.5	53

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127	Ternary behavior and systematic nanoscale manipulation of domain structures in P3HT/PCBM/P3HT-b-PEO films. Journal of Materials Chemistry, 2012, 22, 13013.	6.7	53
128	New insights into the dynamics and morphology of P3HT:PCBM active layers in bulk heterojunctions. Physical Chemistry Chemical Physics, 2013, 15, 17873.	1.3	53
129	Molecular dynamics simulation of twist motion in polyethylene. Macromolecules, 1991, 24, 4148-4151.	2.2	52
130	High Conduction Hopping Behavior Induced in Transition Metal Dichalcogenides by Percolating Defect Networks: Toward Atomically Thin Circuits. Advanced Functional Materials, 2017, 27, 1702829.	7.8	52
131	Diffusion of Sticky Nanoparticles in a Polymer Melt: Crossover from Suppressed to Enhanced Transport. Macromolecules, 2018, 51, 2268-2275.	2.2	52
132	The Role of Sulfur in the Synthesis of Novel Carbon Morphologies: From Covalent Yâ€Junctions to Seaâ€Urchinâ€Like Structures. Advanced Functional Materials, 2009, 19, 1193-1199.	7.8	51
133	Effects of backbone rigidity on the local structure and dynamics in polymer melts and glasses. Physical Chemistry Chemical Physics, 2013, 15, 4604.	1.3	51
134	Tuning interfacial thermal conductance of graphene embedded in soft materials by vacancy defects. Journal of Chemical Physics, 2015, 142, 244703.	1.2	51
135	Dynamic Charge Storage in Ionic Liquids-Filled Nanopores: Insight from a Computational Cyclic Voltammetry Study. Journal of Physical Chemistry Letters, 2015, 6, 22-30.	2.1	51
136	Solid-State Combustion of Metallic Nanoparticles: New Possibilities for an Alternative Energy Carrier. Journal of Energy Resources Technology, Transactions of the ASME, 2007, 129, 29-32.	1.4	50
137	Effect of polymer-filler interaction strengths on the thermodynamic and dynamic properties of polymer nanocomposites. Journal of Chemical Physics, 2009, 130, 134910.	1.2	50
138	New Insights on Electro-Optical Response of Poly(3,4-ethylenedioxythiophene):Poly(styrenesulfonate) Film to Humidity. ACS Applied Materials & Interfaces, 2017, 9, 15880-15886.	4.0	50
139	Size-Expanded yDNA Bases:Â An Ab Initio Study. Journal of Physical Chemistry B, 2006, 110, 6379-6384.	1.2	49
140	Surfactant-Mediated Polyelectrolyte Self-Assembly in a Polyelectrolyteâ€“Surfactant Complex. Macromolecules, 2015, 48, 9050-9059.	2.2	49
141	Automated and Autonomous Experiments in Electron and Scanning Probe Microscopy. ACS Nano, 2021, 15, 12604-12627.	7.3	49
142	Intramolecular vibrational energy flow in model fourâ€atom systems. Journal of Chemical Physics, 1985, 82, 4557-4565.	1.2	48
143	Studies of the intramolecular dynamics of model polyatomic molecules. Journal of Chemical Physics, 1987, 86, 2805-2817.	1.2	48
144	Poly(3-hexylthiophene) Molecular Bottlebrushes via Ring-Opening Metathesis Polymerization: Macromolecular Architecture Enhanced Aggregation. ACS Macro Letters, 2013, 2, 761-765.	2.3	48

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145	Density-fitted singles and doubles coupled cluster on graphics processing units. Molecular Physics, 2014, 112, 844-852.	0.8	48
146	Theoretical Predictions of Freestanding Honeycomb Sheets of Cadmium Chalcogenides. Journal of Physical Chemistry C, 2014, 118, 16236-16245.	1.5	48
147	Electronic Properties of Bilayer Graphene Strongly Coupled to Interlayer Stacking and an External Electric Field. Physical Review Letters, 2015, 115, 015502.	2.9	47
148	A bridge for accelerating materials by design. Npj Computational Materials, 2015, 1, .	3.5	47
149	Oriented Nanostructures from Single Molecules of a Semiconducting Polymer:â€‰ Polarization Evidence for Highly Aligned Intramolecular Geometries. Nano Letters, 2003, 3, 603-607.	4.5	46
150	Mesoscopic Framework Enables Facile Ionic Transport in Solid Electrolytes for Li Batteries. Advanced Energy Materials, 2016, 6, 1600053.	10.2	46
151	Narrow-Bandwidth Spontaneous Luminescence from Oriented Semiconducting Polymer Nanostructures. Journal of Physical Chemistry B, 2003, 107, 6252-6257.	1.2	45
152	Polymer Nanoparticle Superlattices for Organic Photovoltaic Applications. Journal of Physical Chemistry Letters, 2011, 2, 3085-3091.	2.1	45
153	Contribution of restricted rotors to quantum sieving of hydrogen isotopes. Physical Review A, 2001, 64, .	1.0	44
154	Observation of two distinct negative trions in tungsten disulfide monolayers. Physical Review B, 2015, 92, .	1.1	44
155	Selective Tuning of the Electronic Properties of Coaxial Nanocables through Exohedral Doping. Nano Letters, 2007, 7, 2383-2388.	4.5	43
156	Properties of One-Dimensional Molybdenum Nanowires in a Confined Environment. Nano Letters, 2009, 9, 1487-1492.	4.5	43
157	Non-Transition-Metal Catalytic System for N₂ Reduction to NH₃: AÂDensity Functional Theory Study of Al-Doped Graphene. Journal of Physical Chemistry Letters, 2018, 9, 570-576.	2.1	43
158	Neural networks and graph theory as computational tools for predicting polymer properties. Macromolecular Theory and Simulations, 1994, 3, 363-378.	0.6	42
159	Enhanced Phase Segregation Induced by Dipolar Interactions in Polymer Blends. Macromolecules, 2014, 47, 6491-6502.	2.2	42
160	Isotope-Engineering the Thermal Conductivity of Two-Dimensional MoS₂. ACS Nano, 2019, 13, 2481-2489.	7.3	42
161	Charge regulation and local dielectric function in planar polyelectrolyte brushes. Journal of Chemical Physics, 2012, 136, 234901.	1.2	41
162	Modeling solvent evaporation during thin film formation in phase separating polymer mixtures. Soft Matter, 2018, 14, 1833-1846.	1.2	41

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163	Probing Phase-Separation Behavior in Polymer-Blend Microparticles:Â Effects of Particle Size and Polymer Mobility. Macromolecules, 1999, 32, 7183-7189.	2.2	40
164	Structure and Electronic Properties of Edge-Functionalized Armchair Boron Nitride Nanoribbons. Journal of Physical Chemistry C, 2012, 116, 15675-15681.	1.5	40
165	Artificial neural network correction for density-functional tight-binding molecular dynamics simulations. MRS Communications, 2019, 9, 867-873.	0.8	40
166	Understanding How Processing Additives Tune the Nanoscale Morphology of High Efficiency Organic Photovoltaic Blends: From Casting Solution to Spunâ€Cast Thin Film. Advanced Functional Materials, 2014, 24, 6647-6657.	7.8	39
167	Molecular Dynamics Investigation of the Relaxation Mechanism of Entangled Polymers after a Large Step Deformation. ACS Macro Letters, 2018, 7, 190-195.	2.3	39
168	Intramolecular dynamics of the overtoneâ€induced isomerization of methyl isocyanide. Journal of Chemical Physics, 1987, 87, 5809-5819.	1.2	38
169	Unimolecular reaction dynamics of dimethylnitramine. Journal of Chemical Physics, 1988, 88, 6889-6897.	1.2	38
170	Opening Up the Black Box of Artificial Neural Networks. Journal of Chemical Education, 1994, 71, 406.	1.1	38
171	Homogeneous polymer blend microparticles with a tunable refractive index. Optics Letters, 1999, 24, 121.	1.7	38
172	Bright Photoluminescence from the Inner Tubes of â€œPeapodâ€â€Derived Doubleâ€Walled Carbon Nanotubes. Small, 2009, 5, 2678-2682.	5.2	38
173	Tunable morphologies from charged block copolymers. Soft Matter, 2010, 6, 6146.	1.2	38
174	In Situ Formation of Pyridyl-Functionalized Poly(3-hexylthiophene)s via Quenching of the Grignard Metathesis Polymerization: Toward Ligands for Semiconductor Quantum Dots. Chemistry of Materials, 2012, 24, 4459-4467.	3.2	38
175	A Novel and Functional Single-Layer Sheet of ZnSe. ACS Applied Materials & Interfaces, 2015, 7, 1458-1464.	4.0	38
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