Bobby G Sumpter

List of Publications by Year
in descending order

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535 papers	27,017 citations	7568 77 h-index	9589 142 g-index
554 all docs	554 docs citations	554 times ranked	31997 citing authors

#	Article	IF	Citations
1	Quantum theory of electronic excitation and sputtering by transmission electron microscopy. Nanoscale, 2023, 15, 1053-1067.	5.6	5
2	Learning in continuous action space for developing high dimensional potential energy models. Nature Communications, 2022, 13, 368.	12.8	21
3	Dynamic aspects of graphene deformation and fracture from approximate density functional theory. Carbon, 2022, 190, 183-193.	10.3	8
4	A machine learning inversion scheme for determining interaction from scattering. Communications Physics, 2022, 5, .	5.3	9
5	Deep Generative Models for Materials Discovery and Machine Learning-Accelerated Innovation. Frontiers in Materials, 2022, 9, .	2.4	19
6	Small angle scattering of diblock copolymers profiled by machine learning. Journal of Chemical Physics, 2022, 156, 131101.	3.0	3
7	Bridging microscopy with molecular dynamics and quantum simulations: an atomAI based pipeline. Npj Computational Materials, 2022, 8, .	8.7	10
8	From classical to quantum dynamics of atomic and ionic species interacting with graphene and its analogue. Theoretical and Computational Chemistry, 2022, , 61-86.	0.4	0
9	From ground to excited electronic state dynamics of electron and ion irradiated graphene nanomaterials. Theoretical and Computational Chemistry, 2022, , 87-107.	0.4	0
10	Physically Informed Machine Learning Prediction of Electronic Density of States. Chemistry of Materials, 2022, 34, 4848-4855.	6.7	23
11	Understanding the Impacts of Supportâ€“Polymer Interactions on the Dynamics of Poly(ethyleneimine) Confined in Mesoporous SBA-15. Journal of the American Chemical Society, 2022, 144, 11664-11675.	13.7	17
12	Decoding polymer self-dynamics using a two-step approach. Physical Review E, 2022, 106, .	2.1	0
13	Strain-Induced asymmetry and on-site dynamics of silicon defects in graphene. Carbon Trends, 2022, 9, 100189.	3.0	0
14	Nonadiabatic Effects on Defect Diffusion in Silicon-Doped Nanographenes. Nano Letters, 2021, 21, 236-242.	9.1	10
15	Dispersity-Driven Stabilization of Coexisting Morphologies in Asymmetric Diblock Copolymer Thin Films. Macromolecules, 2021, 54, 450-459.	4.8	2
16	An exact inversion method for extracting orientation ordering by small-angle scattering. Physical Chemistry Chemical Physics, 2021, 23, 4120-4132.	2.8	4
17	Machine learned features from density of states for accurate adsorption energy prediction. Nature Communications, 2021, 12, 88.	12.8	108
18	Spatiotemporal mapping of mesoscopic liquid dynamics. Physical Review E, 2021, 103, 022609.	2.1	6

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19	Oxidative Dehydrogenation of Propane to Propylene with Soft Oxidants via Heterogeneous Catalysis. ACS Catalysis, 2021, 11, 2182-2234.	11.2	97
20	MX Anti-MXenes from Non-van der Waals Bulks for Electrochemical Applications: The Merit of Metallicity and Active Basal Plane. ACS Nano, 2021, 15, 6233-6242.	14.6	26
21	Strain in Metal Halide Perovskites: The Critical Role of A-Site Cation. ACS Applied Energy Materials, 2021, 4, 2068-2072.	5.1	14
22	Interactions of an Imine Polymer with Nanoporous Silica and Carbon in Hybrid Adsorbents for Carbon Capture. Langmuir, 2021, 37, 4622-4631.	3.5	7
23	New Insights into the Bulk and Surface Defect Structures of Ceria Nanocrystals from Neutron Scattering Study. Chemistry of Materials, 2021, 33, 3959-3970.	6.7	24
24	Revealing the Chemical Bonding in Adatom Arrays via Machine Learning of Hyperspectral Scanning Tunneling Spectroscopy Data. ACS Nano, 2021, 15, 11806-11816.	14.6	13
25	Benchmarking graph neural networks for materials chemistry. Npj Computational Materials, 2021, 7, .	8.7	113
26	Ensemble learning-iterative training machine learning for uncertainty quantification and automated experiment in atom-resolved microscopy. Npj Computational Materials, 2021, 7, .	8.7	26
27	Automated and Autonomous Experiments in Electron and Scanning Probe Microscopy. ACS Nano, 2021, 15, 12604-12627.	14.6	49
28	Topological Effects Near Orderâ€“Disorder Transitions in Symmetric Diblock Copolymer Melts. Macromolecules, 2021, 54, 7492-7499.	4.8	9
29	Single-atom catalysts with anionic metal centers: Promising electrocatalysts for the oxygen reduction reaction and beyond. Journal of Energy Chemistry, 2021, 63, 285-293.	12.9	15
30	Spatial correlations of entangled polymer dynamics. Physical Review E, 2021, 104, 024503.	2.1	5
31	Electron-Beam-Induced Molecular Plasmon Excitation and Energy Transfer in Silver Molecular Nanowires. Journal of Physical Chemistry A, 2021, 125, 74-87.	2.5	3
32	Mapping the Interfacial Chemistry and Structure of Partially Fluorinated Bottlebrush Polymers and Their Linear Analogues. Langmuir, 2021, 37, 211-218.	3.5	5
33	Tracking atomic structure evolution during directed electron beam induced Si-atom motion in graphene via deep machine learning. Nanotechnology, 2021, 32, 035703.	2.6	10
34	Structural and Dynamical Roles of Bound Polymer Chains in Rubber Reinforcement. Macromolecules, 2021, 54, 11032-11046.	4.8	17
35	On-surface cyclodehydrogenation reaction pathway determined by selective molecular deuterations. Chemical Science, 2021, 12, 15637-15644.	7.4	11
36	Inverse design of two-dimensional materials with invertible neural networks. Npj Computational Materials, 2021, 7, .	8.7	15

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37	Structures of Partially Fluorinated Bottlebrush Polymers in Thin Films. ACS Applied Polymer Materials, 2020, 2, 209-219.	4.4	7
38	Understanding Beam-Induced Electronic Excitations in Materials. Journal of Chemical Theory and Computation, 2020, 16, 1200-1214.	5.3	13
39	Generalized Protein-Repellent Properties of Ultrathin Homopolymer Films. Macromolecules, 2020, 53, 6547-6554.	4.8	5
40	Density-functional tight-binding for phosphine-stabilized nanoscale gold clusters. Chemical Science, 2020, 11, 13113-13128.	7.4	19
41	The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design. Npj Computational Materials, 2020, 6, .	8.7	181
42	Modulating Microphase Separation of Lamellae-Forming Diblock Copolymers via Ionic Junctions. ACS Macro Letters, 2020, 9, 1667-1673.	4.8	9
43	Double membrane formation in heterogeneous vesicles. Soft Matter, 2020, 16, 8806-8817.	2.7	3
44	Improved Single-Ion Conductivity of Polymer Electrolyte via Accelerated Segmental Dynamics. ACS Applied Energy Materials, 2020, 3, 12540-12548.	5.1	31
45	In situ multimodal imaging for nanoscale visualization of tribofilm formation. Journal of Applied Physics, 2020, 127, 154303.	2.5	4
46	Titelbild: Radical Chemistry and Reaction Mechanisms of Propane Oxidative Dehydrogenation over Hexagonal Boron Nitride Catalysts (Angew. Chem. 21/2020). Angewandte Chemie, 2020, 132, 8045-8045.	2.0	0
47	Radical Chemistry and Reaction Mechanisms of Propane Oxidative Dehydrogenation over Hexagonal Boron Nitride Catalysts. Angewandte Chemie - International Edition, 2020, 59, 8042-8046.	13.8	83
48	Radical Chemistry and Reaction Mechanisms of Propane Oxidative Dehydrogenation over Hexagonal Boron Nitride Catalysts. Angewandte Chemie, 2020, 132, 8119-8123.	2.0	11
49	Addition of Short Polymer Chains Mechanically Reinforces Glassy Poly(2-vinylpyridine)â€“Silica Nanoparticle Nanocomposites. ACS Applied Nano Materials, 2020, 3, 3427-3438.	5.0	21
50	Reconstruction of effective potential from statistical analysis of dynamic trajectories. AIP Advances, 2020, 10, .	1.3	4
51	Capacitance of thin films containing polymerized ionic liquids. Science Advances, 2020, 6, eaba7952.	10.3	12
52	Electronic band contraction induced low temperature methane activation on metal alloys. Journal of Materials Chemistry A, 2020, 8, 6057-6066.	10.3	28
53	Strainâ€“Chemical Gradient and Polarization in Metal Halide Perovskites. Advanced Electronic Materials, 2020, 6, 1901235.	5.1	19
54	Electron-beam introduction of heteroatomic Ptâ€“Si structures in graphene. Carbon, 2020, 161, 750-757.	10.3	34

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55	The role of mid-gap phonon modes in thermal transport of transition metal dichalcogenides. Journal of Physics Condensed Matter, 2020, 32, 025306.	1.8	3
56	Understanding the effects of dipolar interactions on the thermodynamics of diblock copolymer melts. Journal of Chemical Physics, 2019, 151, 054902.	3.0	10
57	Multi-Model Imaging of Local Chemistry and Ferroic Properties of Hybrid Organic-Inorganic Perovskites. Microscopy and Microanalysis, 2019, 25, 2076-2077.	0.4	3
58	The influence of curvature on domain distribution in binary mixture membranes. Soft Matter, 2019, 15, 6642-6649.	2.7	5
59	A dicyanobenzoquinone based cathode material for rechargeable lithium and sodium ion batteries. Journal of Materials Chemistry A, 2019, 7, 17888-17895.	10.3	35
60	Artificial neural network correction for density-functional tight-binding molecular dynamics simulations. MRS Communications, 2019, 9, 867-873.	1.8	40
61	Helium Ion Microscopy Imaging of Bottlebrush Copolymers. Microscopy and Microanalysis, 2019, 25, 908-909.	0.4	0
62	Direct Observation of Symmetry-Dependent Electronâ€“Phonon Coupling in Black Phosphorus. Journal of the American Chemical Society, 2019, 141, 18994-19001.	13.7	21
63	Lightâ€Ferroic Interaction in Hybrid Organicâ€“Inorganic Perovskites. Advanced Optical Materials, 2019, 7, 1901451.	7.3	24
64	Protein Resistance Driven by Polymer Nanoarchitecture. ACS Macro Letters, 2019, 8, 1153-1159.	4.8	9
65	Ab initio investigation of the cyclodehydrogenation process for polyanthrylene transformation to graphene nanoribbons. Npj Computational Materials, 2019, 5, .	8.7	9
66	Decoding Liquid Crystal Oligomer Phase Transitions: Toward Molecularly Engineered Shape Changing Materials. Macromolecules, 2019, 52, 6878-6888.	4.8	12
67	Noncontact tip-enhanced Raman spectroscopy for nanomaterials and biomedical applications. Nanoscale Advances, 2019, 1, 3392-3399.	4.6	7
68	Building and exploring libraries of atomic defects in graphene: Scanning transmission electron and scanning tunneling microscopy study. Science Advances, 2019, 5, eaaw8989.	10.3	70
69	Isotope-Engineering the Thermal Conductivity of Two-Dimensional MoS₂. ACS Nano, 2019, 13, 2481-2489.	14.6	42
70	Deep learning analysis of defect and phase evolution during electron beam-induced transformations in WS2. Npj Computational Materials, 2019, 5, .	8.7	113
71	Structural correlations tailor conductive properties in polymerized ionic liquids. Physical Chemistry Chemical Physics, 2019, 21, 14775-14785.	2.8	9
72	Electronically Nonadiabatic Structural Transformations Promoted by Electron Beams. Advanced Functional Materials, 2019, 29, 1901901.	14.9	12

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73	The Fragment Molecular Orbital Method Based on Long-Range Corrected Density-Functional Tight-Binding. Journal of Chemical Theory and Computation, 2019, 15, 3008-3020.	5.3	35
74	Chain conformation of polymer melts with associating groups. Journal of Physics Communications, 2019, 3, 035007.	1.2	10
75	Hierarchical TiO₂:Cu₂O Nanostructures for Gas/Vapor Sensing and CO₂ Sequestration. ACS Applied Materials & Interfaces, 2019, 11, 48466-48475.	8.0	18
76	Lightâ€“Ferroic Interaction: Lightâ€Ferroic Interaction in Hybrid Organicâ€“Inorganic Perovskites (Advanced Optical Materials 23/2019). Advanced Optical Materials, 2019, 7, 1970090.	7.3	1
77	Reply to: On the ferroelectricity of CH3NH3PbI3 perovskites. Nature Materials, 2019, 18, 1051-1053.	27.5	21
78	Design of Atomically Precise Nanoscale Negative Differential Resistance Devices. Advanced Theory and Simulations, 2019, 2, 1800172.	2.8	18
79	Amphiphilic Bottlebrush Block Copolymers: Analysis of Aqueous Self-Assembly by Small-Angle Neutron Scattering and Surface Tension Measurements. Macromolecules, 2019, 52, 465-476.	4.8	56
80	A fast scheme to calculate electronic couplings between P3HT polymer units using diabatic orbitals for charge transfer dynamics simulations. Journal of Computational Chemistry, 2019, 40, 532-542.	3.3	2
81	Prediction of Carbon Dioxide Adsorption via Deep Learning. Angewandte Chemie - International Edition, 2019, 58, 259-263.	13.8	74
82	Direct writing of heterostructures in single atomically precise graphene nanoribbons. Physical Review Materials, 2019, 3, .	2.4	18
83	Theory and Simulation of Attractive Nanoparticle Transport in Polymer Melts. Macromolecules, 2018, 51, 2258-2267.	4.8	38
84	Diffusion of Sticky Nanoparticles in a Polymer Melt: Crossover from Suppressed to Enhanced Transport. Macromolecules, 2018, 51, 2268-2275.	4.8	52
85	Ab Initio Predictions of Strong Interfaces in Transition-Metal Carbides and Nitrides for Superhard Nanocomposite Coating Applications. ACS Applied Nano Materials, 2018, 1, 2029-2035.	5.0	17
86	Anomalous interlayer vibrations in strongly coupled layered PdSe ₂. 2D Materials, 2018, 5, 035016.	4.4	60
87	Interpreting Neutron Reflectivity Profiles of Diblock Copolymer Nanocomposite Thin Films Using Hybrid Particle-Field Simulations. Macromolecules, 2018, 51, 3116-3125.	4.8	4
88	Theoretical investigations of electrical transport properties in CoSb3 skutterudites under hydrostatic loadings. Rare Metals, 2018, 37, 316-325.	7.1	8
89	Bulk and Surface Morphologies of ABC Miktoarm Star Terpolymers Composed of PDMS, PI, and PMMA Arms. Macromolecules, 2018, 51, 1041-1051.	4.8	18
90	Multi-purposed Ar gas cluster ion beam processing for graphene engineering. Carbon, 2018, 131, 142-148.	10.3	18

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91	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.	4.6	43
92	Structure-induced switching of interpolymer adhesion at a solidâ€“polymer melt interface. Soft Matter, 2018, 14, 1108-1119.	2.7	30
93	Modeling solvent evaporation during thin film formation in phase separating polymer mixtures. Soft Matter, 2018, 14, 1833-1846.	2.7	41
94	Molecular Dynamics Investigation of the Relaxation Mechanism of Entangled Polymers after a Large Step Deformation. ACS Macro Letters, 2018, 7, 190-195.	4.8	39
95	A physical catalyst for the electrolysis of nitrogen to ammonia. Science Advances, 2018, 4, e1700336.	10.3	264
96	Adsorption of Molecular Nitrogen in Electrical Double Layers near Planar and Atomically Sharp Electrodes. Langmuir, 2018, 34, 14552-14561.	3.5	2
97	Interphase Structures and Dynamics near Nanofiller Surfaces in Polymer Solutions. Macromolecules, 2018, 51, 9462-9470.	4.8	21
98	Enhanced scattering induced by electrostatic correlations in concentrated solutions of salt-free dipolar and ionic polymers. Journal of Chemical Physics, 2018, 149, 163336.	3.0	8
99	Selectively Deuterated Poly(Îµ-caprolactone)s: Synthesis and Isotope Effects on the Crystal Structures and Properties. Macromolecules, 2018, 51, 9393-9404.	4.8	20
100	Dynamical disparity between hydration shell water and RNA in a hydrated RNA system. Physical Review E, 2018, 98, .	2.1	7
101	Performance of Density-Functional Tight-Binding in Comparison to Ab Initio and First-Principles Methods for Isomer Geometries and Energies of Glucose Epimers in Vacuo and Solution. ACS Omega, 2018, 3, 16899-16915.	3.5	12
102	On the morphological behavior of ABC miktoarm stars containing poly(cis 1,4â€isoprene), poly(styrene), and poly(2â€vinylpyridine). Journal of Polymer Science, Part B: Polymer Physics, 2018, 56, 1491-1504.	2.1	6
103	Theoretical assessment of the nuclear quantum effects on polymer crystallinity via perturbation theory and dynamics. International Journal of Quantum Chemistry, 2018, 118, e25712.	2.0	3
104	Atmospheric and Long-term Aging Effects on the Electrical Properties of Variable Thickness WSe₂ Transistors. ACS Applied Materials & Interfaces, 2018, 10, 36540-36548.	8.0	31
105	Assessing the Predictive Power of Density Functional Theory in Finite-Temperature Hydrogen Adsorption/Desorption Thermodynamics. Journal of Physical Chemistry C, 2018, 122, 26189-26195.	3.1	5
106	Probing static discharge of polymer surfaces with nanoscale resolution. Nanotechnology, 2018, , .	2.6	0
107	Molecular Structure and Dynamics of Interfacial Polymerized Ionic Liquids. Journal of Physical Chemistry C, 2018, 122, 22494-22503.	3.1	8
108	Studies on the 3-Lamellar Morphology of Miktoarm Terpolymers. Macromolecules, 2018, 51, 7491-7499.	4.8	14

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109	Molecular reorganization in bulk bottlebrush polymers: direct observation via nanoscale imaging. Nanoscale, 2018, 10, 18001-18009.	5.6	14
110	Scaling Behavior of Anisotropy Relaxation in Deformed Polymers. Physical Review Letters, 2018, 121, 117801.	7.8	13
111	Theoretical and experimental evidence of conformational transformation in stereoisomers of nucleoside analogues. International Journal of Quantum Chemistry, 2018, 118, e25714.	2.0	0
112	An experimental and computational study of donorâ€“linkerâ€“acceptor block copolymers for organic photovoltaics. Journal of Polymer Science, Part B: Polymer Physics, 2018, 56, 1135-1143.	2.1	4
113	Solvate Ionic Liquids at Electrified Interfaces. ACS Applied Materials & Interfaces, 2018, 10, 32151-32161.	8.0	13
114	Machine learning enabled acoustic detection of sub-nanomolar concentration of trypsin and plasmin in solution. Sensors and Actuators B: Chemical, 2018, 272, 282-288.	7.8	28
115	Molecular blends of methylated-poly(ethylenimine) and amorphous porous organic cages for SO₂ adsorption. Journal of Materials Chemistry A, 2018, 6, 22043-22052.	10.3	24
116	Chemical nature of ferroelastic twin domains in CH3NH3PbI3 perovskite. Nature Materials, 2018, 17, 1013-1019.	27.5	183
117	Light-Activated Hybrid Nanocomposite Film for Water and Oxygen Sensing. ACS Applied Materials & Interfaces, 2018, 10, 31745-31754.	8.0	12
118	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></</r Physical Review Letters, 2018, 121, 086101.	7.8	66
119	Understanding the effects of symmetric salt on the structure of a planar dipolar polymer brush. Journal of Chemical Physics, 2018, 149, 163334.	3.0	3
120	Strain-engineered optoelectronic properties of 2D transition metal dichalcogenide lateral heterostructures. 2D Materials, 2017, 4, 021016.	4.4	72
121	A Computational Approach for Modeling Neutron Scattering Data from Lipid Bilayers. Journal of Chemical Theory and Computation, 2017, 13, 916-925.	5.3	17
122	Unraveling the Agglomeration Mechanism in Charged Block Copolymer and Surfactant Complexes. Macromolecules, 2017, 50, 1193-1205.	4.8	30
123	Aminopolymer functionalization of boron nitride nanosheets for highly efficient capture of carbon dioxide. Journal of Materials Chemistry A, 2017, 5, 16241-16248.	10.3	67
124	Triphasic 2D Materials by Vertically Stacking Laterally Heterostructured 2Hâ€/1Tâ€²â€MoS₂ on Graphene for Enhanced Photoresponse. Advanced Electronic Materials, 2017, 3, 1700024.	5.1	31
125	Linking Silica Support Morphology to the Dynamics of Aminopolymers in Composites. Langmuir, 2017, 33, 5412-5422.	3.5	11
126	New Insights on Electro-Optical Response of Poly(3,4-ethylenedioxythiophene):Poly(styrenesulfonate) Film to Humidity. ACS Applied Materials & Interfaces, 2017, 9, 15880-15886.	8.0	50

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127	Dynamics of Charged Species in Ionic-Neutral Block Copolymer and Surfactant Complexes. Journal of Physical Chemistry B, 2017, 121, 6958-6968.	2.6	9
128	Hydro-deoxygenation of CO on functionalized carbon nanotubes for liquid fuels production. Carbon, 2017, 121, 274-284.	10.3	14
129	Optical signatures of defects in low temperature Raman and photoluminescence spectra of 2D crystals (Conference Presentation). , 2017, , .		0
130	Ultrafast charge and energy exchanges at hybrid interfaces involving 2D semiconductors (Conference) Tj ETQq0 0 0 rgBT /Overlock 10 T		0
131	Enhancing Ion Migration in Grain Boundaries of Hybrid Organicâ€“Inorganic Perovskites by Chlorine. Advanced Functional Materials, 2017, 27, 1700749.	14.9	74
132	Aminopolymer Mobility and Support Interactions in Silica-PEI Composites for CO₂ Capture Applications: A Quasielastic Neutron Scattering Study. Journal of Physical Chemistry B, 2017, 121, 6721-6731.	2.6	30
133	Multicomponent Gas Storage in Organic Cage Molecules. Journal of Physical Chemistry C, 2017, 121, 12426-12433.	3.1	15
134	A Rayleighian approach for modeling kinetics of ionic transport in polymeric media. Journal of Chemical Physics, 2017, 146, 064902.	3.0	12
135	An automated analysis workflow for optimization of force-field parameters using neutron scattering data. Journal of Computational Physics, 2017, 340, 128-137.	3.8	10
136	Focus: Structure and dynamics of the interfacial layer in polymer nanocomposites with attractive interactions. Journal of Chemical Physics, 2017, 146, 203201.	3.0	114
137	Nanoporous poly(3-hexylthiophene) thin film structures from self-organization of a tunable molecular bottlebrush scaffold. Nanoscale, 2017, 9, 7071-7080.	5.6	18
138	Controllable conversion of quasi-freestanding polymer chains to graphene nanoribbons. Nature Communications, 2017, 8, 14815.	12.8	58
139	Interfacial Properties of Polymer Nanocomposites: Role of Chain Rigidity and Dynamic Heterogeneity Length Scale. Macromolecules, 2017, 50, 2397-2406.	4.8	115
140	Investigations on the Phase Diagram and Interaction Parameter of Poly(styrene-b-1,3-cyclohexadiene) Copolymers. Macromolecules, 2017, 50, 2354-2363.	4.8	5
141	Emerging materials for lowering atmospheric carbon. Environmental Technology and Innovation, 2017, 7, 30-43.	6.1	13
142	Big Effect of Small Nanoparticles: A Shift in Paradigm for Polymer Nanocomposites. ACS Nano, 2017, 11, 752-759.	14.6	177
143	Ab Initio Predictions of Hexagonal Zr(B,C,N) Polymorphs for Coherent Interface Design. Journal of Physical Chemistry C, 2017, 121, 26007-26018.	3.1	9
144	Ionic liquids-mediated interactions between nanorods. Journal of Chemical Physics, 2017, 147, 134704.	3.0	2

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145	Interlayer bond polarizability model for stacking-dependent low-frequency Raman scattering in layered materials. Nanoscale, 2017, 9, 15340-15355.	5.6	38
146	Relevance of the Nuclear Quantum Effects on the Proton/Deuteron Transmission through Hexagonal Boron Nitride and Graphene Monolayers. Journal of Physical Chemistry C, 2017, 121, 24335-24344.	3.1	23
147	Deuteration as a Means to Tune Crystallinity of Conducting Polymers. Journal of Physical Chemistry Letters, 2017, 8, 4333-4340.	4.6	16
148	Building with ions: towards direct write of platinum nanostructures using in situ liquid cell helium ion microscopy. Nanoscale, 2017, 9, 12949-12956.	5.6	8
149	Effects of counterion size and backbone rigidity on the dynamics of ionic polymer melts and glasses. Physical Chemistry Chemical Physics, 2017, 19, 27442-27451.	2.8	22
150	Multi-mode humidity sensing with water-soluble copper phthalocyanine for increased sensitivity and dynamic range. Scientific Reports, 2017, 7, 9921.	3.3	17
151	PdSe₂: Pentagonal Two-Dimensional Layers with High Air Stability for Electronics. Journal of the American Chemical Society, 2017, 139, 14090-14097.	13.7	509
152	Perovskites: Enhancing Ion Migration in Grain Boundaries of Hybrid Organicâ€“Inorganic Perovskites by Chlorine (Adv. Funct. Mater. 26/2017). Advanced Functional Materials, 2017, 27, .	14.9	1
153	Attraction between Opposing Planar Dipolar Polymer Brushes. Langmuir, 2017, 33, 9231-9240.	3.5	7
154	UV-activated ZnO films on a flexible substrate for room temperature O2 and H2O sensing. Scientific Reports, 2017, 7, 6053.	3.3	61
155	High Conduction Hopping Behavior Induced in Transition Metal Dichalcogenides by Percolating Defect Networks: Toward Atomically Thin Circuits. Advanced Functional Materials, 2017, 27, 1702829.	14.9	52
156	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.	2.6	82
157	Low-Frequency Shear and Layer-Breathing Modes in Raman Scattering of Two-Dimensional Materials. ACS Nano, 2017, 11, 11777-11802.	14.6	179
158	Effects of partial La filling and Sb vacancy defects on <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>CoS</mml:mi><mml:msub><mml:mi mathvariant="normal">b</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> skutterudites. Physical Review B, 2017, 95, .	3.2	26
159	Isomeric effects on the self-assembly of a plausible prebiotic nucleoside analogue: A theoretical study. International Journal of Quantum Chemistry, 2017, 117, 213-221.	2.0	2
160	Noncovalent Interactions in Nanotechnology. , 2017, , 417-451.		8
161	Engineering the Bacterial Microcompartment Domain for Molecular Scaffolding Applications. Frontiers in Microbiology, 2017, 8, 1441.	3.5	57
162	Development and Modeling of a Novel Self-Assembly Process for Polymer and Polymeric Composite Nanoparticles. , 2017, , 143-176.		0

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163	Monomer volume fraction profiles in pH responsive planar polyelectrolyte brushes. Journal of Polymer Science, Part B: Polymer Physics, 2016, 54, 956-964.	2.1	28
164	Thermodynamics and Kinetics of Gas Storage in Porous Liquids. Journal of Physical Chemistry B, 2016, 120, 7195-7200.	2.6	64
165	Grain boundary stability and influence on ionic conductivity in a disordered perovskiteâ€"a first-principles investigation of lithium lanthanum titanate. MRS Communications, 2016, 6, 455-463.	1.8	11
166	Supramolecular polymerization of a prebiotic nucleoside provides insights into the creation of sequence-controlled polymers. Scientific Reports, 2016, 6, 18891.	3.3	5
167	Directing Matter: Toward Atomic-Scale 3D Nanofabrication. ACS Nano, 2016, 10, 5600-5618.	14.6	99
168	PEDOT:PSS/QCM-based multimodal humidity and pressure sensor. Sensors and Actuators B: Chemical, 2016, 236, 91-98.	7.8	58
169	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.	11.2	116
170	Thermoreversible Morphology and Conductivity of a Conjugated Polymer Network Embedded in Block Copolymer Selfâ€Assemblies. Small, 2016, 12, 4857-4864.	10.0	5
171	Highâ€Selectivity Electrochemical Conversion of CO₂ to Ethanol using a Copper Nanoparticle/Nâ€Doped Graphene Electrode. ChemistrySelect, 2016, 1, 6055-6061.	1.5	251
172	Thermodynamic Control of Two-Dimensional Molecular Ionic Nanostructures on Metal Surfaces. ACS Nano, 2016, 10, 7821-7829.	14.6	8
173	Understanding How Isotopes Affect Charge Transfer in P3HT/PCBM: A Quantum Trajectory-Electronic Structure Study with Nonlinear Quantum Corrections. Journal of Chemical Theory and Computation, 2016, 12, 4487-4500.	5.3	11
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