

Bobby G Sumpter

List of Publications by Year in descending order

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535
papers

27,017
citations

7551

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h-index

9553

142
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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. <i>Nanoscale</i> , 2023, 15, 1053-1067.	2.8	5
2	Learning in continuous action space for developing high dimensional potential energy models. <i>Nature Communications</i> , 2022, 13, 368.	5.8	21
3	Dynamic aspects of graphene deformation and fracture from approximate density functional theory. <i>Carbon</i> , 2022, 190, 183-193.	5.4	8
4	A machine learning inversion scheme for determining interaction from scattering. <i>Communications Physics</i> , 2022, 5, .	2.0	9
5	Deep Generative Models for Materials Discovery and Machine Learning-Accelerated Innovation. <i>Frontiers in Materials</i> , 2022, 9, .	1.2	19
6	Small angle scattering of diblock copolymers profiled by machine learning. <i>Journal of Chemical Physics</i> , 2022, 156, 131101.	1.2	3
7	Bridging microscopy with molecular dynamics and quantum simulations: an atomAI based pipeline. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	10
8	From classical to quantum dynamics of atomic and ionic species interacting with graphene and its analogue. <i>Theoretical and Computational Chemistry</i> , 2022, , 61-86.	0.2	0
9	From ground to excited electronic state dynamics of electron and ion irradiated graphene nanomaterials. <i>Theoretical and Computational Chemistry</i> , 2022, , 87-107.	0.2	0
10	Physically Informed Machine Learning Prediction of Electronic Density of States. <i>Chemistry of Materials</i> , 2022, 34, 4848-4855.	3.2	23
11	Understanding the Impacts of Support-Polymer Interactions on the Dynamics of Poly(ethyleneimine) Confined in Mesoporous SBA-15. <i>Journal of the American Chemical Society</i> , 2022, 144, 11664-11675.	6.6	17
12	Decoding polymer self-dynamics using a two-step approach. <i>Physical Review E</i> , 2022, 106, .	0.8	0
13	Strain-Induced asymmetry and on-site dynamics of silicon defects in graphene. <i>Carbon Trends</i> , 2022, 9, 100189.	1.4	0
14	Nonadiabatic Effects on Defect Diffusion in Silicon-Doped Nanographenes. <i>Nano Letters</i> , 2021, 21, 236-242.	4.5	10
15	Dispersy-Driven Stabilization of Coexisting Morphologies in Asymmetric Diblock Copolymer Thin Films. <i>Macromolecules</i> , 2021, 54, 450-459.	2.2	2
16	An exact inversion method for extracting orientation ordering by small-angle scattering. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4120-4132.	1.3	4
17	Machine learned features from density of states for accurate adsorption energy prediction. <i>Nature Communications</i> , 2021, 12, 88.	5.8	108
18	Spatiotemporal mapping of mesoscopic liquid dynamics. <i>Physical Review E</i> , 2021, 103, 022609.	0.8	6

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19	Oxidative Dehydrogenation of Propane to Propylene with Soft Oxidants via Heterogeneous Catalysis. ACS Catalysis, 2021, 11, 2182-2234.	5.5	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.	7.3	26
21	Strain in Metal Halide Perovskites: The Critical Role of A-Site Cation. ACS Applied Energy Materials, 2021, 4, 2068-2072.	2.5	14
22	Interactions of an Imine Polymer with Nanoporous Silica and Carbon in Hybrid Adsorbents for Carbon Capture. Langmuir, 2021, 37, 4622-4631.	1.6	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.	3.2	24
24	Revealing the Chemical Bonding in Adatom Arrays via Machine Learning of Hyperspectral Scanning Tunneling Spectroscopy Data. ACS Nano, 2021, 15, 11806-11816.	7.3	13
25	Benchmarking graph neural networks for materials chemistry. Npj Computational Materials, 2021, 7, .	3.5	113
26	Ensemble learning-iterative training machine learning for uncertainty quantification and automated experiment in atom-resolved microscopy. Npj Computational Materials, 2021, 7, .	3.5	26
27	Automated and Autonomous Experiments in Electron and Scanning Probe Microscopy. ACS Nano, 2021, 15, 12604-12627.	7.3	49
28	Topological Effects Near Order-Disorder Transitions in Symmetric Diblock Copolymer Melts. Macromolecules, 2021, 54, 7492-7499.	2.2	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.	7.1	15
30	Spatial correlations of entangled polymer dynamics. Physical Review E, 2021, 104, 024503.	0.8	5
31	Electron-Beam-Induced Molecular Plasmon Excitation and Energy Transfer in Silver Molecular Nanowires. Journal of Physical Chemistry A, 2021, 125, 74-87.	1.1	3
32	Mapping the Interfacial Chemistry and Structure of Partially Fluorinated Bottlebrush Polymers and Their Linear Analogues. Langmuir, 2021, 37, 211-218.	1.6	5
33	Tracking atomic structure evolution during directed electron beam induced Si-atom motion in graphene via deep machine learning. Nanotechnology, 2021, 32, 035703.	1.3	10
34	Structural and Dynamical Roles of Bound Polymer Chains in Rubber Reinforcement. Macromolecules, 2021, 54, 11032-11046.	2.2	17
35	On-surface cyclodehydrogenation reaction pathway determined by selective molecular deuterations. Chemical Science, 2021, 12, 15637-15644.	3.7	11
36	Inverse design of two-dimensional materials with invertible neural networks. Npj Computational Materials, 2021, 7, .	3.5	15

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37	Structures of Partially Fluorinated Bottlebrush Polymers in Thin Films. <i>ACS Applied Polymer Materials</i> , 2020, 2, 209-219.	2.0	7
38	Understanding Beam-Induced Electronic Excitations in Materials. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1200-1214.	2.3	13
39	Generalized Protein-Repellent Properties of Ultrathin Homopolymer Films. <i>Macromolecules</i> , 2020, 53, 6547-6554.	2.2	5
40	Density-functional tight-binding for phosphine-stabilized nanoscale gold clusters. <i>Chemical Science</i> , 2020, 11, 13113-13128.	3.7	19
41	The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	181
42	Modulating Microphase Separation of Lamellae-Forming Diblock Copolymers via Ionic Junctions. <i>ACS Macro Letters</i> , 2020, 9, 1667-1673.	2.3	9
43	Double membrane formation in heterogeneous vesicles. <i>Soft Matter</i> , 2020, 16, 8806-8817.	1.2	3
44	Improved Single-Ion Conductivity of Polymer Electrolyte via Accelerated Segmental Dynamics. <i>ACS Applied Energy Materials</i> , 2020, 3, 12540-12548.	2.5	31
45	In situ multimodal imaging for nanoscale visualization of tribofilm formation. <i>Journal of Applied Physics</i> , 2020, 127, 154303.	1.1	4
46	Titelbild: Radical Chemistry and Reaction Mechanisms of Propane Oxidative Dehydrogenation over Hexagonal Boron Nitride Catalysts (<i>Angew. Chem.</i> 21/2020). <i>Angewandte Chemie</i> , 2020, 132, 8045-8045.	1.6	0
47	Radical Chemistry and Reaction Mechanisms of Propane Oxidative Dehydrogenation over Hexagonal Boron Nitride Catalysts. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 8042-8046.	7.2	83
48	Radical Chemistry and Reaction Mechanisms of Propane Oxidative Dehydrogenation over Hexagonal Boron Nitride Catalysts. <i>Angewandte Chemie</i> , 2020, 132, 8119-8123.	1.6	11
49	Addition of Short Polymer Chains Mechanically Reinforces Glassy Poly(2-vinylpyridine)-Silica Nanoparticle Nanocomposites. <i>ACS Applied Nano Materials</i> , 2020, 3, 3427-3438.	2.4	21
50	Reconstruction of effective potential from statistical analysis of dynamic trajectories. <i>AIP Advances</i> , 2020, 10, .	0.6	4
51	Capacitance of thin films containing polymerized ionic liquids. <i>Science Advances</i> , 2020, 6, eaba7952.	4.7	12
52	Electronic band contraction induced low temperature methane activation on metal alloys. <i>Journal of Materials Chemistry A</i> , 2020, 8, 6057-6066.	5.2	28
53	Strain-Chemical Gradient and Polarization in Metal Halide Perovskites. <i>Advanced Electronic Materials</i> , 2020, 6, 1901235.	2.6	19
54	Electron-beam introduction of heteroatomic Pt-Si structures in graphene. <i>Carbon</i> , 2020, 161, 750-757.	5.4	34

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55	The role of mid-gap phonon modes in thermal transport of transition metal dichalcogenides. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 025306.	0.7	3
56	Understanding the effects of dipolar interactions on the thermodynamics of diblock copolymer melts. <i>Journal of Chemical Physics</i> , 2019, 151, 054902.	1.2	10
57	Multi-Model Imaging of Local Chemistry and Ferroc Properties of Hybrid Organic-Inorganic Perovskites. <i>Microscopy and Microanalysis</i> , 2019, 25, 2076-2077.	0.2	3
58	The influence of curvature on domain distribution in binary mixture membranes. <i>Soft Matter</i> , 2019, 15, 6642-6649.	1.2	5
59	A dicyanobenzoquinone based cathode material for rechargeable lithium and sodium ion batteries. <i>Journal of Materials Chemistry A</i> , 2019, 7, 17888-17895.	5.2	35
60	Artificial neural network correction for density-functional tight-binding molecular dynamics simulations. <i>MRS Communications</i> , 2019, 9, 867-873.	0.8	40
61	Helium Ion Microscopy Imaging of Bottlebrush Copolymers. <i>Microscopy and Microanalysis</i> , 2019, 25, 908-909.	0.2	0
62	Direct Observation of Symmetry-Dependent Electron-Phonon Coupling in Black Phosphorus. <i>Journal of the American Chemical Society</i> , 2019, 141, 18994-19001.	6.6	21
63	Light-Ferroc Interaction in Hybrid Organic-Inorganic Perovskites. <i>Advanced Optical Materials</i> , 2019, 7, 1901451.	3.6	24
64	Protein Resistance Driven by Polymer Nanoarchitecture. <i>ACS Macro Letters</i> , 2019, 8, 1153-1159.	2.3	9
65	Ab initio investigation of the cyclodehydrogenation process for polyanthrylene transformation to graphene nanoribbons. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	9
66	Decoding Liquid Crystal Oligomer Phase Transitions: Toward Molecularly Engineered Shape Changing Materials. <i>Macromolecules</i> , 2019, 52, 6878-6888.	2.2	12
67	Noncontact tip-enhanced Raman spectroscopy for nanomaterials and biomedical applications. <i>Nanoscale Advances</i> , 2019, 1, 3392-3399.	2.2	7
68	Building and exploring libraries of atomic defects in graphene: Scanning transmission electron and scanning tunneling microscopy study. <i>Science Advances</i> , 2019, 5, eaaw8989.	4.7	70
69	Isotope-Engineering the Thermal Conductivity of Two-Dimensional MoS ₂ . <i>ACS Nano</i> , 2019, 13, 2481-2489.	7.3	42
70	Deep learning analysis of defect and phase evolution during electron beam-induced transformations in WS ₂ . <i>Npj Computational Materials</i> , 2019, 5, .	3.5	113
71	Structural correlations tailor conductive properties in polymerized ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14775-14785.	1.3	9
72	Electronically Nonadiabatic Structural Transformations Promoted by Electron Beams. <i>Advanced Functional Materials</i> , 2019, 29, 1901901.	7.8	12

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73	The Fragment Molecular Orbital Method Based on Long-Range Corrected Density-Functional Tight-Binding. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3008-3020.	2.3	35
74	Chain conformation of polymer melts with associating groups. <i>Journal of Physics Communications</i> , 2019, 3, 035007.	0.5	10
75	Hierarchical TiO ₂ :Cu ₂ O Nanostructures for Gas/Vapor Sensing and CO ₂ Sequestration. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 48466-48475.	4.0	18
76	Light-Induced Ferroic Interaction in Hybrid Organic-Inorganic Perovskites (Advanced Optical Materials 23/2019). <i>Advanced Optical Materials</i> , 2019, 7, 1970090.	3.6	1
77	Reply to: On the ferroelectricity of CH ₃ NH ₃ PbI ₃ perovskites. <i>Nature Materials</i> , 2019, 18, 1051-1053.	13.3	21
78	Design of Atomically Precise Nanoscale Negative Differential Resistance Devices. <i>Advanced Theory and Simulations</i> , 2019, 2, 1800172.	1.3	18
79	Amphiphilic Bottlebrush Block Copolymers: Analysis of Aqueous Self-Assembly by Small-Angle Neutron Scattering and Surface Tension Measurements. <i>Macromolecules</i> , 2019, 52, 465-476.	2.2	56
80	A fast scheme to calculate electronic couplings between P3HT polymer units using diabatic orbitals for charge transfer dynamics simulations. <i>Journal of Computational Chemistry</i> , 2019, 40, 532-542.	1.5	2
81	Prediction of Carbon Dioxide Adsorption via Deep Learning. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 259-263.	7.2	74
82	Direct writing of heterostructures in single atomically precise graphene nanoribbons. <i>Physical Review Materials</i> , 2019, 3, .	0.9	18
83	Theory and Simulation of Attractive Nanoparticle Transport in Polymer Melts. <i>Macromolecules</i> , 2018, 51, 2258-2267.	2.2	38
84	Diffusion of Sticky Nanoparticles in a Polymer Melt: Crossover from Suppressed to Enhanced Transport. <i>Macromolecules</i> , 2018, 51, 2268-2275.	2.2	52
85	Ab Initio Predictions of Strong Interfaces in Transition-Metal Carbides and Nitrides for Superhard Nanocomposite Coating Applications. <i>ACS Applied Nano Materials</i> , 2018, 1, 2029-2035.	2.4	17
86	Anomalous interlayer vibrations in strongly coupled layered PdSe ₂ . <i>2D Materials</i> , 2018, 5, 035016.	2.0	60
87	Interpreting Neutron Reflectivity Profiles of Diblock Copolymer Nanocomposite Thin Films Using Hybrid Particle-Field Simulations. <i>Macromolecules</i> , 2018, 51, 3116-3125.	2.2	4
88	Theoretical investigations of electrical transport properties in CoSb ₃ skutterudites under hydrostatic loadings. <i>Rare Metals</i> , 2018, 37, 316-325.	3.6	8
89	Bulk and Surface Morphologies of ABC Miktoarm Star Terpolymers Composed of PDMS, PI, and PMMA Arms. <i>Macromolecules</i> , 2018, 51, 1041-1051.	2.2	18
90	Multi-purposed Ar gas cluster ion beam processing for graphene engineering. <i>Carbon</i> , 2018, 131, 142-148.	5.4	18

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91	Non-Transition-Metal Catalytic System for N ₂ Reduction to NH ₃ : A Density Functional Theory Study of Al-Doped Graphene. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 570-576.	2.1	43
92	Structure-induced switching of interpolymer adhesion at a solid-polymer melt interface. <i>Soft Matter</i> , 2018, 14, 1108-1119.	1.2	30
93	Modeling solvent evaporation during thin film formation in phase separating polymer mixtures. <i>Soft Matter</i> , 2018, 14, 1833-1846.	1.2	41
94	Molecular Dynamics Investigation of the Relaxation Mechanism of Entangled Polymers after a Large Step Deformation. <i>ACS Macro Letters</i> , 2018, 7, 190-195.	2.3	39
95	A physical catalyst for the electrolysis of nitrogen to ammonia. <i>Science Advances</i> , 2018, 4, e1700336.	4.7	264
96	Adsorption of Molecular Nitrogen in Electrical Double Layers near Planar and Atomically Sharp Electrodes. <i>Langmuir</i> , 2018, 34, 14552-14561.	1.6	2
97	Interphase Structures and Dynamics near Nanofiller Surfaces in Polymer Solutions. <i>Macromolecules</i> , 2018, 51, 9462-9470.	2.2	21
98	Enhanced scattering induced by electrostatic correlations in concentrated solutions of salt-free dipolar and ionic polymers. <i>Journal of Chemical Physics</i> , 2018, 149, 163336.	1.2	8
99	Selectively Deuterated Poly(ϵ -caprolactone)s: Synthesis and Isotope Effects on the Crystal Structures and Properties. <i>Macromolecules</i> , 2018, 51, 9393-9404.	2.2	20
100	Dynamical disparity between hydration shell water and RNA in a hydrated RNA system. <i>Physical Review E</i> , 2018, 98, .	0.8	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. <i>ACS Omega</i> , 2018, 3, 16899-16915.	1.6	12
102	On the morphological behavior of ABC miktoarm stars containing poly(cis 1,4-isoprene), poly(styrene), and poly(2-vinylpyridine). <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2018, 56, 1491-1504.	2.4	6
103	Theoretical assessment of the nuclear quantum effects on polymer crystallinity via perturbation theory and dynamics. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25712.	1.0	3
104	Atmospheric and Long-term Aging Effects on the Electrical Properties of Variable Thickness WSe ₂ Transistors. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 36540-36548.	4.0	31
105	Assessing the Predictive Power of Density Functional Theory in Finite-Temperature Hydrogen Adsorption/Desorption Thermodynamics. <i>Journal of Physical Chemistry C</i> , 2018, 122, 26189-26195.	1.5	5
106	Probing static discharge of polymer surfaces with nanoscale resolution. <i>Nanotechnology</i> , 2018, , .	1.3	0
107	Molecular Structure and Dynamics of Interfacial Polymerized Ionic Liquids. <i>Journal of Physical Chemistry C</i> , 2018, 122, 22494-22503.	1.5	8
108	Studies on the 3-Lamellar Morphology of Miktoarm Terpolymers. <i>Macromolecules</i> , 2018, 51, 7491-7499.	2.2	14

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109	Molecular reorganization in bulk bottlebrush polymers: direct observation <i>via</i> nanoscale imaging. <i>Nanoscale</i> , 2018, 10, 18001-18009.	2.8	14
110	Scaling Behavior of Anisotropy Relaxation in Deformed Polymers. <i>Physical Review Letters</i> , 2018, 121, 117801.	2.9	13
111	Theoretical and experimental evidence of conformational transformation in stereoisomers of nucleoside analogues. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25714.	1.0	0
112	An experimental and computational study of donor-linker-acceptor block copolymers for organic photovoltaics. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2018, 56, 1135-1143.	2.4	4
113	Solvate Ionic Liquids at Electrified Interfaces. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 32151-32161.	4.0	13
114	Machine learning enabled acoustic detection of sub-nanomolar concentration of trypsin and plasmin in solution. <i>Sensors and Actuators B: Chemical</i> , 2018, 272, 282-288.	4.0	28
115	Molecular blends of methylated-poly(ethylenimine) and amorphous porous organic cages for SO ₂ adsorption. <i>Journal of Materials Chemistry A</i> , 2018, 6, 22043-22052.	5.2	24
116	Chemical nature of ferroelastic twin domains in CH ₃ NH ₃ PbI ₃ perovskite. <i>Nature Materials</i> , 2018, 17, 1013-1019.	13.3	183
117	Light-Activated Hybrid Nanocomposite Film for Water and Oxygen Sensing. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 31745-31754.	4.0	12
118	3D Imaging and Manipulation of Subsurface Selenium Vacancies in PdSe_2 . <i>Physical Review Letters</i> , 2018, 121, 086101.	2.9	66
119	Understanding the effects of symmetric salt on the structure of a planar dipolar polymer brush. <i>Journal of Chemical Physics</i> , 2018, 149, 163334.	1.2	3
120	Strain-engineered optoelectronic properties of 2D transition metal dichalcogenide lateral heterostructures. <i>2D Materials</i> , 2017, 4, 021016.	2.0	72
121	A Computational Approach for Modeling Neutron Scattering Data from Lipid Bilayers. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 916-925.	2.3	17
122	Unraveling the Agglomeration Mechanism in Charged Block Copolymer and Surfactant Complexes. <i>Macromolecules</i> , 2017, 50, 1193-1205.	2.2	30
123	Aminopolymer functionalization of boron nitride nanosheets for highly efficient capture of carbon dioxide. <i>Journal of Materials Chemistry A</i> , 2017, 5, 16241-16248.	5.2	67
124	Triphasic 2D Materials by Vertically Stacking Laterally Heterostructured 2H-TaC ₂ /MoS ₂ on Graphene for Enhanced Photoresponse. <i>Advanced Electronic Materials</i> , 2017, 3, 1700024.	2.6	31
125	Linking Silica Support Morphology to the Dynamics of Aminopolymers in Composites. <i>Langmuir</i> , 2017, 33, 5412-5422.	1.6	11
126	New Insights on Electro-Optical Response of Poly(3,4-ethylenedioxythiophene):Poly(styrenesulfonate) Film to Humidity. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 15880-15886.	4.0	50

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127	Dynamics of Charged Species in Ionic-Neutral Block Copolymer and Surfactant Complexes. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6958-6968.	1.2	9
128	Hydro-deoxygenation of CO on functionalized carbon nanotubes for liquid fuels production. <i>Carbon</i> , 2017, 121, 274-284.	5.4	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 /Ovgrlock 10 T		
131	Enhancing Ion Migration in Grain Boundaries of Hybrid Organic-Inorganic Perovskites by Chlorine. <i>Advanced Functional Materials</i> , 2017, 27, 1700749.	7.8	74
132	Aminopolymer Mobility and Support Interactions in Silica-PEI Composites for CO ₂ Capture Applications: A Quasielastic Neutron Scattering Study. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6721-6731.	1.2	30
133	Multicomponent Gas Storage in Organic Cage Molecules. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12426-12433.	1.5	15
134	A Rayleighian approach for modeling kinetics of ionic transport in polymeric media. <i>Journal of Chemical Physics</i> , 2017, 146, 064902.	1.2	12
135	An automated analysis workflow for optimization of force-field parameters using neutron scattering data. <i>Journal of Computational Physics</i> , 2017, 340, 128-137.	1.9	10
136	Focus: Structure and dynamics of the interfacial layer in polymer nanocomposites with attractive interactions. <i>Journal of Chemical Physics</i> , 2017, 146, 203201.	1.2	114
137	Nanoporous poly(3-hexylthiophene) thin film structures from self-organization of a tunable molecular bottlebrush scaffold. <i>Nanoscale</i> , 2017, 9, 7071-7080.	2.8	18
138	Controllable conversion of quasi-freestanding polymer chains to graphene nanoribbons. <i>Nature Communications</i> , 2017, 8, 14815.	5.8	58
139	Interfacial Properties of Polymer Nanocomposites: Role of Chain Rigidity and Dynamic Heterogeneity Length Scale. <i>Macromolecules</i> , 2017, 50, 2397-2406.	2.2	115
140	Investigations on the Phase Diagram and Interaction Parameter of Poly(styrene- <i>b</i> -1,3-cyclohexadiene) Copolymers. <i>Macromolecules</i> , 2017, 50, 2354-2363.	2.2	5
141	Emerging materials for lowering atmospheric carbon. <i>Environmental Technology and Innovation</i> , 2017, 7, 30-43.	3.0	13
142	Big Effect of Small Nanoparticles: A Shift in Paradigm for Polymer Nanocomposites. <i>ACS Nano</i> , 2017, 11, 752-759.	7.3	177
143	Ab Initio Predictions of Hexagonal Zr(B,C,N) Polymorphs for Coherent Interface Design. <i>Journal of Physical Chemistry C</i> , 2017, 121, 26007-26018.	1.5	9
144	Ionic liquids-mediated interactions between nanorods. <i>Journal of Chemical Physics</i> , 2017, 147, 134704.	1.2	2

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145	Interlayer bond polarizability model for stacking-dependent low-frequency Raman scattering in layered materials. <i>Nanoscale</i> , 2017, 9, 15340-15355.	2.8	38
146	Relevance of the Nuclear Quantum Effects on the Proton/Deuteron Transmission through Hexagonal Boron Nitride and Graphene Monolayers. <i>Journal of Physical Chemistry C</i> , 2017, 121, 24335-24344.	1.5	23
147	Deuteration as a Means to Tune Crystallinity of Conducting Polymers. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4333-4340.	2.1	16
148	Building with ions: towards direct write of platinum nanostructures using in situ liquid cell helium ion microscopy. <i>Nanoscale</i> , 2017, 9, 12949-12956.	2.8	8
149	Effects of counterion size and backbone rigidity on the dynamics of ionic polymer melts and glasses. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 27442-27451.	1.3	22
150	Multi-mode humidity sensing with water-soluble copper phthalocyanine for increased sensitivity and dynamic range. <i>Scientific Reports</i> , 2017, 7, 9921.	1.6	17
151	PdSe ₂ : Pentagonal Two-Dimensional Layers with High Air Stability for Electronics. <i>Journal of the American Chemical Society</i> , 2017, 139, 14090-14097.	6.6	509
152	Perovskites: Enhancing Ion Migration in Grain Boundaries of Hybrid Organic-Inorganic Perovskites by Chlorine (Adv. Funct. Mater. 26/2017). <i>Advanced Functional Materials</i> , 2017, 27, .	7.8	1
153	Attraction between Opposing Planar Dipolar Polymer Brushes. <i>Langmuir</i> , 2017, 33, 9231-9240.	1.6	7
154	UV-activated ZnO films on a flexible substrate for room temperature O ₂ and H ₂ O sensing. <i>Scientific Reports</i> , 2017, 7, 6053.	1.6	61
155	High Conduction Hopping Behavior Induced in Transition Metal Dichalcogenides by Percolating Defect Networks: Toward Atomically Thin Circuits. <i>Advanced Functional Materials</i> , 2017, 27, 1702829.	7.8	52
156	Influence of Chain Rigidity and Dielectric Constant on the Glass Transition Temperature in Polymerized Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2017, 121, 11511-11519.	1.2	82
157	Low-Frequency Shear and Layer-Breathing Modes in Raman Scattering of Two-Dimensional Materials. <i>ACS Nano</i> , 2017, 11, 11777-11802.	7.3	179
158	Effects of partial La filling and Sb vacancy defects on CoS_3 skutterudites. <i>Physical Review B</i> , 2017, 95, .	1.1	26
159	Isomeric effects on the self-assembly of a plausible prebiotic nucleoside analogue: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2017, 117, 213-221.	1.0	2
160	Noncovalent Interactions in Nanotechnology. , 2017, , 417-451.		8
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