Seung Soon Jang

List of Publications by Year
in descending order

171 papers	6,563 citations	66343 42 h-index	76900 74 g-index
172 all docs	172 docs citations	172 times ranked	8186 citing authors

#	Article	IF	Citations
1	Nanophase-Segregation and Transport in Nafion 117 from Molecular Dynamics Simulations:Â Effect of Monomeric Sequence. Journal of Physical Chemistry B, 2004, 108, 3149-3157.	2.6	425
2	Low-temperature solution-processed Li-doped SnO2 as an effective electron transporting layer for high-performance flexible and wearable perovskite solar cells. Nano Energy, 2016, 26, 208-215.	16.0	419
3	Self-polymerized dopamine as an organic cathode for Li- and Na-ion batteries. Energy and Environmental Science, 2017, 10, 205-215.	30.8	253
4	Molecular Dynamics Study of a Surfactant-Mediated Decaneâ^'Water Interface:â€‰ Effect of Molecular Architecture of Alkyl Benzene Sulfonate. Journal of Physical Chemistry B, 2004, 108, 12130-12140.	2.6	244
5	Collagen intrafibrillar mineralization as a result of the balance between osmotic equilibrium and electroneutrality. Nature Materials, 2017, 16, 370-378.	27.5	210
6	Structures and Properties of Self-Assembled Monolayers of Bistable [2]Rotaxanes on Au (111) Surfaces from Molecular Dynamics Simulations Validated with Experiment. Journal of the American Chemical Society, 2005, 127, 1563-1575.	13.7	202
7	First-Principles Density Functional Theory Modeling of Li Binding: Thermodynamics and Redox Properties of Quinone Derivatives for Lithium-Ion Batteries. Journal of the American Chemical Society, 2016, 138, 2374-2382.	13.7	194
8	All Solid-State Lithium Batteries Assembled with Hybrid Solid Electrolytes. Journal of the Electrochemical Society, 2015, 162, A704-A710.	2.9	158
9	Mechanical and Transport Properties of the Poly(ethylene oxide)â^'Poly(acrylic acid) Double Network Hydrogel from Molecular Dynamic Simulations. Journal of Physical Chemistry B, 2007, 111, 1729-1737.	2.6	142
10	Multi-paradigm multi-scale simulations for fuel cell catalysts and membranes. Molecular Simulation, 2006, 32, 251-268.	2.0	117
11	The Source of Helicity in PerfluorinatedN-Alkanes. Macromolecules, 2003, 36, 5331-5341.	4.8	108
12	Structures and Properties of Newton Black Films Characterized Using Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 7992-8001.	2.6	103
13	Molecular Dynamics Simulation of Amphiphilic Bistable [2]Rotaxane Langmuir Monolayers at the Air/Water Interface. Journal of the American Chemical Society, 2005, 127, 14804-14816.	13.7	102
14	Application of DFT-based machine learning for developing molecular electrode materials in Li-ion batteries. RSC Advances, 2018, 8, 39414-39420.	3.6	96
15	Aromatic Ionomers with Highly Acidic Sulfonate Groups: Acidity, Hydration, and Proton Conductivity. Macromolecules, 2011, 44, 8458-8469.	4.8	90
16	ReaxFF Reactive Force Field for Solid Oxide Fuel Cell Systems with Application to Oxygen Ion Transport in Yttria-Stabilized Zirconia. Journal of Physical Chemistry A, 2008, 112, 3133-3140.	2.5	88
17	Molecular Dynamics Simulation Study of a Polysulfone-Based Anion Exchange Membrane in Comparison with the Proton Exchange Membrane. Journal of Physical Chemistry C, 2014, 118, 12577-12587.	3.1	84
18	â€œOrganic Aqua Regiaâ€â€”Powerful Liquids for Dissolving Noble Metals. Angewandte Chemie - International Edition, 2010, 49, 7929-7932.	13.8	82

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19	Adsorption of Î²-d-glucose and cellobiose on kaolinite surfaces: Density functional theory (DFT) approach. Applied Clay Science, 2013, 71, 73-81.	5.2	78
20	High-Density Lithium-Ion Energy Storage Utilizing the Surface Redox Reactions in Folded Graphene Films. Chemistry of Materials, 2015, 27, 3291-3298.	6.7	78
21	Density Functional Theory Studies of the [2]Rotaxane Component of the Stoddartâ^'Heath Molecular Switch. Journal of the American Chemical Society, 2004, 126, 12636-12645.	13.7	74
22	Molecular dynamics simulation study of P (VP-co-HEMA) hydrogels: Effect of water content on equilibrium structures and mechanical properties. Biomaterials, 2009, 30, 6130-6141.	11.4	73
23	First-Principles Study of the Switching Mechanism of [2]Catenane Molecular Electronic Devices. Physical Review Letters, 2005, 94, 156801.	7.8	72
24	Innovative cathode flow-field design for passive air-cooled polymer electrolyte membrane (PEM) fuel cell stacks. International Journal of Hydrogen Energy, 2020, 45, 11704-11713.	7.1	72
25	Magnetism in Dopant-Free ZnO Nanoplates. Nano Letters, 2012, 12, 576-581.	9.1	64
26	Water distribution in dentin matrices: Bound vs. unbound water. Dental Materials, 2015, 31, 205-216.	3.5	63
27	Nanophase Segregation and Water Dynamics in the Dendrion Diblock Copolymer Formed from the FrÃ©chet Polyaryl Ethereal Dendrimer and Linear PTFE. Journal of Physical Chemistry B, 2005, 109, 10154-10167.	2.6	62
28	Polymer electrolyte membranes based on poly(arylene ether sulfone) with pendant perfluorosulfonic acid. Polymer Chemistry, 2013, 4, 272-281.	3.9	61
29	Structure Solution from Powder Diffraction of Copper 1,4â€Benzenedicarboxylate. European Journal of Inorganic Chemistry, 2014, 2014, 2140-2145.	2.0	59
30	The importance of size-exclusion characteristics of type I collagen in bonding to dentin matrices. Acta Biomaterialia, 2013, 9, 9522-9528.	8.3	58
31	Effect of Superacidic Side Chain Structures on High Conductivity Aromatic Polymer Fuel Cell Membranes. Macromolecules, 2015, 48, 7117-7126.	4.8	57
32	Lead-free halide double perovskites: Toward stable and sustainable optoelectronic devices. Materials Today, 2021, 49, 123-144.	14.2	57
33	Role of anions on electrochemical exfoliation of graphite into graphene in aqueous acids. Carbon, 2020, 167, 816-825.	10.3	54
34	Structures and Transport Properties of Hydrated Water-Soluble Dendrimer-Grafted Polymer Membranes for Application to Polymer Electrolyte Membrane Fuel Cells:â€‰ Classical Molecular Dynamics Approach. Journal of Physical Chemistry C, 2007, 111, 2759-2769.	3.1	51
35	A molecular dynamics simulation study of hydrated sulfonated poly(ether ether ketone) for application to polymer electrolyte membrane fuel cells: Effect of water content. Journal of Renewable and Sustainable Energy, 2009, 1, .	2.0	51
36	First-principles study of Li adsorption in a carbon nanotube-fullerene hybrid system. Carbon, 2011, 49, 286-293.	10.3	51

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37	Cytoprotective Self-assembled RGD Peptide Nanofilms for Surface Modification of Viable Mesenchymal Stem Cells. Chemistry of Materials, 2017, 29, 2055-2065.	6.7	51
38	Interfacial Reactions of Ozone with Surfactant Protein B in a Model Lung Surfactant System. Journal of the American Chemical Society, 2010, 132, 2254-2263.	13.7	49
39	Monte Carlo simulation of the orderâ€“disorder transition of a symmetric cyclic diblock copolymer system. Journal of Chemical Physics, 1999, 111, 1712-1720.	3.0	48
40	Molecular Dynamics Simulation Study on a Monolayer of Half [2]Rotaxane Self-Assembled on Au(111). Journal of the American Chemical Society, 2005, 127, 4959-4964.	13.7	45
41	Effect of cyclic chain architecture on properties of dilute solutions of polyethylene from molecular dynamics simulations. Journal of Chemical Physics, 2003, 119, 1843-1854.	3.0	44
42	Conformations and charge transport characteristics of biphenyldithiol self-assembled-monolayer molecular electronic devices: A multiscale computational study. Journal of Chemical Physics, 2005, 122, 244703.	3.0	44
43	Molecular dynamics simulation study of sodium dodecyl sulfate micelle: Water penetration and sodium dodecyl sulfate dissociation. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2015, 474, 36-43.	4.7	44
44	Molecular Dynamics Simulations of Aldol Condensation Catalyzed by Alkylamine-Functionalized Crystalline Silica Surfaces. Journal of the American Chemical Society, 2016, 138, 7664-7672.	13.7	44
45	Systematic Molecular Design of Ketone Derivatives of Aromatic Molecules for Lithiumâ€Ion Batteries: Firstâ€Principles DFT Modeling. ChemSusChem, 2017, 10, 1584-1591.	6.8	44
46	Effect of monomeric sequence on nanostructure and water dynamics in Nafion 117. Solid State Ionics, 2004, 175, 805-808.	2.7	42
47	Importance of Exsolution in Transition-Metal (Co, Rh, and Ir)-Doped LaCrO₃ Perovskite Catalysts for Boosting Dry Reforming of CH₄ Using CO₂ for Hydrogen Production. Industrial & Engineering Chemistry Research, 2019, 58, 6385-6393.	3.7	41
48	Effect of ZnO nanoparticles morphology on UV blocking of poly(vinyl alcohol)/ZnO composite nanofibers. Materials Letters, 2015, 147, 20-24.	2.6	39
49	Thermodynamic and redox properties of graphene oxides for lithium-ion battery applications: a first principles density functional theory modeling approach. Physical Chemistry Chemical Physics, 2016, 18, 20600-20606.	2.8	39
50	Free Energy Barrier for Molecular Motions in Bistable [2]Rotaxane Molecular Electronic Devices. Journal of Physical Chemistry A, 2009, 113, 2136-2143.	2.5	38
51	Interaction of C₆₀ with Water: First-Principles Modeling and Environmental Implications. Environmental Science & Technology, 2015, 49, 1529-1536.	10.0	37
52	Electrochemical Properties of Boronâ€Doped Fullerene Derivatives for Lithiumâ€Ion Battery Applications. ChemPhysChem, 2018, 19, 753-758.	2.1	37
53	Electrochemical and electronic properties of nitrogen doped fullerene and its derivatives for lithium-ion battery applications. Journal of Energy Chemistry, 2018, 27, 528-534.	12.9	36
54	Analyzing oxygen transport resistance and Pt particle growth effect in the cathode catalyst layer of polymer electrolyte fuel cells. International Journal of Hydrogen Energy, 2020, 45, 13414-13427.	7.1	35

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55	Effect of Monomeric Sequence on Mechanical Properties of P(VP-co-HEMA) Hydrogels at Low Hydration. Journal of Physical Chemistry B, 2009, 113, 6604-6612.	2.6	34
56	Cycling performance of lithium-ion polymer cells assembled with a cross-linked composite polymer electrolyte using a fibrous polyacrylonitrile membrane and vinyl-functionalized SiO₂ nanoparticles. Journal of Materials Chemistry A, 2015, 3, 12163-12170.	10.3	34
57	Preparation of poly(ethylene terephthalate-co-isophthalate) by ester interchange reaction in the PET/PEI blend system. Journal of Polymer Science, Part B: Polymer Physics, 1997, 35, 309-315.	2.1	32
58	A density functional theory (DFT) study of CO2 adsorption on Mg-rich minerals by enhanced charge distribution. Computational Materials Science, 2014, 95, 181-186.	3.0	32
59	Adsorption of carboxylate on calcium carbonate (1 0 4) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 602 Td (surface: Molecular simulation approach. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2015, 474, 9-17.	4.7	32
60	Unveiled correlations between electron affinity and solvation in redox potential of quinone-based sodium-ion batteries. Energy Storage Materials, 2019, 19, 242-250.	18.0	32
61	Nanostructures of Nafion Film at Platinum/Carbon Surface in Catalyst Layer of PEMFC: Molecular Dynamics Simulation Approach. Journal of Physical Chemistry C, 2020, 124, 21386-21395.	3.1	32
62	Interactions of Pt nanoparticles with molecular components in polymer electrolyte membrane fuel cells: multi-scale modeling approach. RSC Advances, 2016, 6, 69670-69676.	3.6	31
63	Covalent organic frameworks: Design and applications in electrochemical energy storage devices. InformaÄnÂ-MateriÃ¡ly, 2022, 4, .	17.3	31
64	Analysis of the mechanical behavior of poly(trimethylene terephthalate) in an amorphous state under uniaxial extensionâ€“compression condition through atomistic modeling. Journal of Chemical Physics, 1999, 110, 7524-7532.	3.0	30
65	Stability of Water-Stable C₆₀Clusters to OH Radical Oxidation and Hydrated Electron Reduction. Environmental Science & Technology, 2010, 44, 3786-3792.	10.0	30
66	Deswelling Mechanisms of Surface-Grafted Poly(NIPAAm) Brush: Molecular Dynamics Simulation Approach. Journal of Physical Chemistry C, 2012, 116, 15974-15985.	3.1	30
67	Activity-stability benefits of Pt/C fuel cell electrocatalysts prepared via remote CeO2 interfacial doping. Journal of Power Sources, 2021, 496, 229798.	7.8	30
68	Mechanism of Li Adsorption on Carbon Nanotube-Fullerene Hybrid System: A First-Principles Study. ACS Applied Materials & Interfaces, 2011, 3, 1186-1194.	8.0	29
69	A Firstâ€Principles Study of Lithium Adsorption on a Grapheneâ€“Fullerene Nanohybrid System. ChemPhysChem, 2015, 16, 789-795.	2.1	29
70	Mechanical and Transport Properties of the Poly(ethylene oxide)â^Poly(acrylic acid) Double Network Hydrogel from Molecular Dynamic Simulations. Journal of Physical Chemistry B, 2007, 111, 14440-14440.	2.6	28
71	Li adsorption on a grapheneâ€“fullerene nanobud system: density functional theory approach. RSC Advances, 2015, 5, 32819-32825.	3.6	27
72	Density Functional Theory â€“ Machine Learning Approach to Analyze the Bandgap of Elemental Halide Perovskites and Ruddlesdenâ€Popper Phases. ChemPhysChem, 2018, 19, 2559-2565.	2.1	27

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73	Molecular structureâ€“redox potential relationship for organic electrode materials: density functional theoryâ€“Machine learning approach. Materials Today Energy, 2020, 17, 100482.	4.7	26
74	Effect of temperature on structure and water transport of hydrated sulfonated poly(ether ether) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 7 2011, 3, .	2.0	25
75	Molecular Modeling Approach to Determine the Floryâ€Huggins Interaction Parameter for Polymer Miscibility Analysis. ChemPhysChem, 2018, 19, 1655-1664.	2.1	24
76	Distribution and Diffusion of Water in Model Epoxy Molding Compound: Molecular Dynamics Simulation Approach. IEEE Transactions on Advanced Packaging, 2010, 33, 333-339.	1.6	23
77	Negative Differential Resistance of Oligo(Phenylene Ethynylene) Self-Assembled Monolayer Systems: The Electric-Field-Induced Conformational Change Mechanism. Journal of Physical Chemistry C, 2011, 115, 3722-3730.	3.1	23
78	Investigation of ethanol infiltration into demineralized dentin collagen fibrils using molecular dynamics simulations. Acta Biomaterialia, 2016, 36, 175-185.	8.3	23
79	Boron-doped coronenes with high redox potential for organic positive electrodes in lithium-ion batteries: a first-principles density functional theory modeling study. Journal of Materials Chemistry A, 2018, 6, 10111-10120.	10.3	22
80	Contiguous and Atomically Thin Pt Film with Supraâ€Bulk Behavior Through Grapheneâ€Imposed Epitaxy. Advanced Functional Materials, 2019, 29, 1902274.	14.9	22
81	Parametric study of passive air-cooled polymer electrolyte membrane fuel cell stacks. International Journal of Heat and Mass Transfer, 2020, 156, 119886.	4.8	22
82	Metal-foam-based cathode flow-field design to improve H2O retention capability of passive air cooled polymer electrolyte fuel cells. International Journal of Thermal Sciences, 2021, 161, 106702.	4.9	21
83	Density Functional Theory Modeling-Assisted Investigation of Thermodynamics and Redox Properties of Boron-Doped Corannulenes for Cathodes in Lithium-Ion Batteries. Journal of Physical Chemistry C, 2018, 122, 10675-10681.	3.1	20
84	Toward enhanced CO2 adsorption on bimodal calcium-based materials with porous truncated architectures. Applied Surface Science, 2020, 505, 144512.	6.1	20
85	Porous Strained Pt Nanostructured Thinâ€Film Electrocatalysts via Dealloying for PEM Fuel Cells. Advanced Materials Interfaces, 2020, 7, 1901326.	3.7	19
86	Investigations of the band structures of edge-defect zigzag graphene nanoribbons using density functional theory. RSC Advances, 2016, 6, 39587-39594.	3.6	18
87	Origin and Control of Polyacrylonitrile Alignments on Carbon Nanotubes and Graphene Nanoribbons. Advanced Functional Materials, 2018, 28, 1706970.	14.9	18
88	CeO₂(111) Surface with Oxygen Vacancy for Radical Scavenging: A Density Functional Theory Approach. Journal of Physical Chemistry C, 2020, 124, 20950-20959.	3.1	18
89	Effect of the Side-Chain Length in Perfluorinated Sulfonic and Phosphoric Acid-Based Membranes on Nanophase Segregation and Transport: A Molecular Dynamics Simulation Approach. Journal of Physical Chemistry B, 2020, 124, 1571-1580.	2.6	18
90	Enhanced Lithium Storage of an Organic Cathode via the Bipolar Mechanism. ACS Applied Energy Materials, 2020, 3, 3728-3735.	5.1	18

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91	Spectral Instability of Layered Mixed Halide Perovskites Results from Anion Phase Redistribution and Selective Hole Injection. ACS Nano, 2021, 15, 1486-1496.	14.6	18
92	Antioxidant technology for durability enhancement in polymer electrolyte membranes for fuel cell applications. Materials Today, 2022, 58, 135-163.	14.2	18
93	Effects of Ester Interchange Reactions on the Phase Behavior of an Immiscible Polyester Blend:Â Monte Carlo Simulation. Macromolecules, 1999, 32, 1679-1685.	4.8	17
94	Li adsorption on a Fullereneâ€“Single wall carbon nanotube hybrid system: Density functional theory approach. Current Applied Physics, 2014, 14, 1748-1754.	2.4	17
95	Controlling the Physicochemical State of Carbon on Graphene Using Focused Electron-Beam-Induced Deposition. ACS Nano, 2014, 8, 6805-6813.	14.6	17
96	Detecting the functional complexities between high-density lipoprotein mimetics. Biomaterials, 2018, 170, 58-69.	11.4	17
97	A hydrogen storage nanotank: lithium-organic pillared graphite. Chemical Communications, 2009, , 5427.	4.1	16
98	Effect of solvent on electrical conductivity and gas sensitivity of PEDOT: PSS polymer composite films. Journal of Applied Polymer Science, 2015, 132, .	2.6	16
99	Monte Carlo simulation of copolymerization by ester interchange reaction in miscible polyester blends. Journal of Polymer Science, Part B: Polymer Physics, 1998, 36, 1637-1645.	2.1	15
100	Functionalized Fullerenes in Water: A Closer Look. Environmental Science & Technology, 2015, 49, 2147-2155.	10.0	15
101	DFT-Machine Learning Approach for Accurate Prediction of pK_a. Journal of Physical Chemistry A, 2021, 125, 8712-8722.	2.5	15
102	Characterization of molecular association of poly(2-oxazoline)s-based micelles with various epoxides and diols via the Floryâ€“Huggins theory: a molecular dynamics simulation approach. Physical Chemistry Chemical Physics, 2015, 17, 29161-29170.	2.8	14
103	Investigation of the effect of erythrosine B on amyloid beta peptide using molecular modeling. Journal of Molecular Modeling, 2016, 22, 92.	1.8	14
104	The effects of ethanol on the size-exclusion characteristics of type I dentin collagen to adhesive resin monomers. Acta Biomaterialia, 2016, 33, 235-241.	8.3	14
105	Enhanced Selectivity for CO₂ Adsorption on Mesoporous Silica with Alkali Metal Halide Due to Electrostatic Field: A Molecular Simulation Approach. ACS Applied Materials & Interfaces, 2017, 9, 31683-31690.	8.0	14
106	Boosting activity toward oxygen reduction reaction of a mesoporous FeCuNC catalyst via heteroatom doping-induced electronic state modulation. Journal of Materials Chemistry A, 2022, 10, 5361-5372.	10.3	14
107	Analysis of the mechanical behavior of amorphous atactic poly(oxypropylene) by atomistic modeling. Macromolecular Theory and Simulations, 1999, 8, 1-9.	1.4	13
108	Influence of SWNTs on the Preferential Alignment of Molecular Moieties in PVA Fibers. Macromolecular Chemistry and Physics, 2012, 213, 617-626.	2.2	13

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109	Thermodynamic Stability of Zimmerman Self-Assembled Dendritic Supramolecules from Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2004, 108, 10041-10052.	2.6	12
110	Effect of monomeric sequence on transport properties of d-glucose and ascorbic acid in poly(VP-co-HEMA) hydrogels with various water contents: molecular dynamics simulation approach. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	12
111	Dynamic modulation of electronic properties of graphene by localized carbon doping using focused electron beam induced deposition. Nanoscale, 2015, 7, 14946-14952.	5.6	12
112	Activating â€œInvisibleâ€•Glue: Using Electron Beam for Enhancement of Interfacial Properties of Grapheneâ€“Metal Contact. ACS Nano, 2016, 10, 1042-1049.	14.6	12
113	Charge Transport through Polyene Self-Assembled Monolayers from Multiscale Computer Simulations. Journal of Physical Chemistry B, 2008, 112, 14888-14897.	2.6	11
114	Localized conductive patterning via focused electron beam reduction of graphene oxide. Applied Physics Letters, 2015, 106, .	3.3	11
115	Density Functional Theory Study of Oxygen Reduction on Graphene and Platinum Surfaces of Ptâ€“Graphene Hybrids. ACS Applied Nano Materials, 2021, 4, 1067-1075.	5.0	11
116	Accelerating Solvent Selection for Type II Porous Liquids. Journal of the American Chemical Society, 2022, 144, 4071-4079.	13.7	11
117	Off-lattice Monte Carlo simulation of hyperbranched polymers, 1 Polycondensation of AB2 type monomers. Macromolecular Theory and Simulations, 2000, 9, 188-195.	1.4	10
118	Phase transformation of poly(trimethylene terephthalate) in crystalline state: An atomistic modeling approach. Fibers and Polymers, 2000, 1, 18-24.	2.1	10
119	Sponge Behaviors of Functionalized Few-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 14868-14875.	3.1	10
120	Possible performance improvement in [2]catenane molecular electronic switches. Applied Physics Letters, 2006, 88, 163112.	3.3	9
121	Effect of Temperature on Water Molecules in a Model Epoxy Molding Compound: Molecular Dynamics Simulation Approach. IEEE Transactions on Components, Packaging and Manufacturing Technology, 2011, 1, 1533-1542.	2.5	9
122	Bandgap bowing in Ta-W-O system for efficient solar energy conversion: Insights from density functional theory and X-ray diffraction. Applied Physics Letters, 2013, 103, 133905.	3.3	9
123	Dissipative particle dynamics simulation study of poly(2-oxazoline)-based multicompartment micelle nanoreactor. Physical Chemistry Chemical Physics, 2016, 18, 6284-6290.	2.8	9
124	Molecular Simulation Study on Factors Affecting Carbon Dioxide Adsorption on Amorphous Silica Surfaces. Journal of Physical Chemistry C, 2020, 124, 12580-12588.	3.1	9
125	Distribution characteristics of phosphoric acid and PTFE binder on Pt/C surfaces in high-temperature polymer electrolyte membrane fuel cells: Molecular dynamics simulation approach. International Journal of Hydrogen Energy, 2021, 46, 17295-17305.	7.1	9
126	Improving Water Management and Performance of an Air-Cooled Fuel Cell System Using Pressurized Air for Aviation Applications. Journal of the Electrochemical Society, 2021, 168, 084503.	2.9	9

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127	Sodium Diffusion through Aluminum-Doped Zeolite BEA System: Effect of Water Solvation. Journal of Physical Chemistry C, 2009, 113, 819-826.	3.1	8
128	Distribution and Transport of CO2 in Hydrated Hyperbranched Poly(ethylenimine) Membranes: A Molecular Dynamics Simulation Approach. ACS Omega, 2021, 6, 3390-3398.	3.5	8
129	One-pot synthesis of linear triblock terpolymers and their aqueous self-assembly. Polymer Chemistry, 2021, 12, 1967-1974.	3.9	8
130	Multi-Variate Optimization of Polymer Electrolyte Membrane Fuel Cells in Consideration of Effects of GDL Compression and Intrusion. Journal of the Electrochemical Society, 2022, 169, 014511.	2.9	8
131	Cooperativity in the Aldol Condensation Using Bifunctional Mesoporous Silicaâ€“Poly(styrene) MCM-41 Organic/Inorganic Hybrid Catalysts. ACS Applied Materials & Interfaces, 2022, 14, 11235-11247.	8.0	8
132	Dissipative particle dynamics simulation of multicompartment micelle nanoreactor with channel for reactants. RSC Advances, 2018, 8, 37866-37871.	3.6	7
133	Structural Tunability of Multicompartment Micelles as a Function of Lipophilicâ€“Fluorophilic Block Length Ratio. Journal of Physical Chemistry B, 2018, 122, 12164-12172.	2.6	7
134	Effect of Block Length and Side Chain Length Ratios on Determining a Multicompartment Micelle Structure. Journal of Physical Chemistry B, 2019, 123, 4784-4791.	2.6	7
135	Creation of discrete active site domains via mesoporous silica poly(styrene) composite materials for incompatible acidâ€“base cascade reactions. Catalysis Science and Technology, 2021, 11, 1311-1322.	4.1	7
136	Tailored Design of Electrochemically Degradable Anthraquinone Functionality toward Organic Cathodes. ACS Applied Materials & Interfaces, 2021, 13, 35729-35738.	8.0	7
137	Effect of Uniaxial Deformation on Structure and Transport in Hydrated Nafion 117: Molecular Dynamics Simulation Study. Materials Performance and Characterization, 2015, 4, 131-147.	0.3	7
138	Porous carbon fibers from gel-spun polyacrylonitrile and poly(methyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 302 Td (methacrylate)-block	10.3	7
139	Singleâ€Step Fabrication of Polymeric Composite Membrane via Centrifugal Colloidal Casting for Fuel Cell Applications. Small Methods, 2021, 5, e2100285.	8.6	6
140	CO2-Selective Zeolitic Imidazolate Framework Membrane on Graphene Oxide Nanoribbons: Experimental and Theoretical Studies. Journal of Materials Chemistry A, 0, , .	10.3	6
141	Tailorâ€Made Charged Catecholâ€Based Polymeric Ligands to Build Robust Fuel Cells Containing Antioxidative Nanoparticles. Advanced Electronic Materials, 2022, 8, .	5.1	6
142	Yielding and plastic behaviour of amorphous atactic poly(oxypropylene) under uniaxial compression: an atomistic modeling approach. Polymer, 1999, 40, 919-925.	3.8	5
143	A mechanistic study of the interaction of water-soluble borate glass with apatite-bound heterocyclic nitrogen-containing bisphosphonates. Acta Biomaterialia, 2016, 31, 339-347.	8.3	5
144	Ce(III)â€Based Coordinationâ€Complexâ€Based Efficient Radical Scavenger for Exceptional Durability Enhancement of Polymer Application in Protonâ€Exchange Membrane Fuel Cells and Organic Photovoltaics. Advanced Energy and Sustainability Research, 2022, 3, .	5.8	5

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145	Homogenization process caused by competition between phase separation and ester-interchange reactions in immiscible polyester blends: A Monte Carlo simulation. Journal of Polymer Science, Part B: Polymer Physics, 2000, 38, 590-598.	2.1	4
146	Synthesis of temporarily solubilised azo disperse dyes containing a Î²â€sulphatoethylsulphonyl group and dispersantâ€free dyeing of polyethylene terephthalate fabric. Coloration Technology, 2016, 132, 368-375.	1.5	4
147	Molecular dynamics simulation study on the structural properties of poly (ethylene terephthalate) under uniaxial extension and thermal shrinkage processes. Current Applied Physics, 2018, 18, 19-26.	2.4	4
148	Group Vibrational Mode Assignments as a Broadly Applicable Tool for Characterizing Ionomer Membrane Structure as a Function of Degree of Hydration. Chemistry of Materials, 2020, 32, 1828-1843.	6.7	4
149	Electron-Transport Characteristics through Aluminum Oxide (100) and (012) in a Metalâ€“Insulatorâ€“Metal Junction System: Density Functional Theoryâ”€Nonequilibrium Green Function Approach. ACS Omega, 2020, 5, 1717-1724.	3.5	4
150	Structural Transformation of a Multicompartment Micelle Induced by Photo-Switchable Spiropyranâ€“Merocyanine Transition: Dissipative Particle Dynamics Simulation Approach. Journal of Physical Chemistry B, 2022, 126, 4401-4410.	2.6	4
151	Structural and Electronic Properties of Sulfuric Acid-Doped Single-Walled Carbon Nanotube. Journal of Computational and Theoretical Nanoscience, 2010, 7, 232-236.	0.4	3
152	Dispersant-free dyeing of poly(lactic acid) fabric with temporarily solubilised disperse dyes from azopyridone derivatives. Coloration Technology, 2016, 132, 361-367.	1.5	2
153	Blends of poly(3-alkylthiophene) and [6,6]-phenyl-C61-butyric acid methyl ester for organic photovoltaic cell applications: Multi-scale modeling approach. Computational Materials Science, 2017, 126, 299-307.	3.0	2
154	Effects of thermal shrinkage temperatures and comonomers on thermal shrinkage of uniaxially-stretched PET copolymer films: a molecular dynamics simulation approach. New Journal of Chemistry, 2018, 42, 4991-4997.	2.8	2
155	Carbon Fibers: Origin and Control of Polyacrylonitrile Alignments on Carbon Nanotubes and Graphene Nanoribbons (Adv. Funct. Mater. 15/2018). Advanced Functional Materials, 2018, 28, 1870099.	14.9	2
156	Multi-Scale First-Principles Modeling of Three-Phase System of Polymer Electrolyte Membrane Fuel Cell. ECS Transactions, 2013, 50, 155-160.	0.5	1
157	Structure and hydrophilicity of azoâ€dyeâ€derived rotaxane: density functional theory approach. Coloration Technology, 2017, 133, 382-390.	1.5	1
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