Seung Soon Jang

List of Publications by Year in Descending Order

153 papers	4,976 citations	38 h-index	65 g-index
172 ext. papers	5,769 ext. citations	6.9 avg, IF	5.77 L-index

#	Paper	IF	Citations
153	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	3.9	0
152	Porous carbon fibers from gel-spun polyacrylonitrile and poly(methyl methacrylate)-block-poly(acrylonitrile). *Carbon*, **2022**, 192, 332-346	10.4	1
151	Spectral Instability of Layered Mixed Halide Perovskites Results from Anion Phase Redistribution and Selective Hole Injection. *ACS Nano*, **2021**, 15, 1486-1496	16.7	8
150	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	6.7	3
149	Activity-stability benefits of Pt/C fuel cell electrocatalysts prepared via remote CeO2 interfacial doping. *Journal of Power Sources*, **2021**, 496, 229798	8.9	2
148	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	4.1	8
147	Creation of discrete active site domains via mesoporous silica poly(styrene) composite materials for incompatible acid–base cascade reactions. *Catalysis Science and Technology*, **2021**, 11, 1311-1322	5.5	3
146	Distribution and Transport of CO in Hydrated Hyperbranched Poly(ethylenimine) Membranes: A Molecular Dynamics Simulation Approach. *ACS Omega*, **2021**, 6, 3390-3398	3.9	2
145	Lead-free halide double perovskites: Toward stable and sustainable optoelectronic devices. *Materials Today*, **2021**,	21.8	16
144	Tailored Design of Electrochemically Degradable Anthraquinone Functionality toward Organic Cathodes. *ACS Applied Materials & Interfaces*, **2021**, 13, 35729-35738	9.5	1
143	Single-Step Fabrication of Polymeric Composite Membrane via Centrifugal Colloidal Casting for Fuel Cell Applications.. *Small Methods*, **2021**, 5, e2100285	12.8	2
142	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	3.9	2
141	DFT-Machine Learning Approach for Accurate Prediction of p. *Journal of Physical Chemistry A*, **2021**, 125, 8712-8722	2.8	1
140	One-pot synthesis of linear triblock terpolymers and their aqueous self-assembly. *Polymer Chemistry*, **2021**, 12, 1967-1974	4.9	1
139	Density Functional Theory Study of Oxygen Reduction on Graphene and Platinum Surfaces of Pt□raphene Hybrids. *ACS Applied Nano Materials*, **2021**, 4, 1067-1075	5.6	2
138	Molecular Simulation Study on Factors Affecting Carbon Dioxide Adsorption on Amorphous Silica Surfaces. *Journal of Physical Chemistry C*, **2020**, 124, 12580-12588	3.8	5
137	Parametric study of passive air-cooled polymer electrolyte membrane fuel cell stacks. *International Journal of Heat and Mass Transfer*, **2020**, 156, 119886	4.9	11

136	Role of anions on electrochemical exfoliation of graphite into graphene in aqueous acids. *Carbon*, **2020**, 167, 816-825	10.4	27
135	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	3.4	9
134	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	9.6	2
133	Electron-Transport Characteristics through Aluminum Oxide (100) and (012) in a Metal-Insulator-Metal Junction System: Density Functional Theory-Nonequilibrium Green Function Approach. *ACS Omega*, **2020**, 5, 1717-1724	3.9	3
132	Enhanced Lithium Storage of an Organic Cathode via the Bipolar Mechanism. *ACS Applied Energy Materials*, **2020**, 3, 3728-3735	6.1	12
131	Toward enhanced CO2 adsorption on bimodal calcium-based materials with porous truncated architectures. *Applied Surface Science*, **2020**, 505, 144512	6.7	8
130	Porous Strained Pt Nanostructured Thin-Film Electrocatalysts via Dealloying for PEM Fuel Cells. *Advanced Materials Interfaces*, **2020**, 7, 1901326	4.6	14
129	Molecular structure–redox potential relationship for organic electrode materials: density functional theory–Machine learning approach. *Materials Today Energy*, **2020**, 17, 100482	7	8
128	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	3.8	11
127	CeO2(111) Surface with Oxygen Vacancy for Radical Scavenging: A Density Functional Theory Approach. *Journal of Physical Chemistry C*, **2020**, 124, 20950-20959	3.8	6
126	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	6.7	26
125	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	6.7	9
124	Effect of Block Length and Side Chain Length Ratios on Determining a Multicompartment Micelle Structure. *Journal of Physical Chemistry B*, **2019**, 123, 4784-4791	3.4	3
123	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	3.9	26
122	Contiguous and Atomically Thin Pt Film with Supra-Bulk Behavior Through Graphene-Imposed Epitaxy. *Advanced Functional Materials*, **2019**, 29, 1902274	15.6	13
121	51.3: Invited Paper: Perovskite Light Emitters via Dimensional and Structural Control. *Digest of Technical Papers SID International Symposium*, **2019**, 50, 568-568	0.5	
120	Unveiled correlations between electron affinity and solvation in redox potential of quinone-based sodium-ion batteries. *Energy Storage Materials*, **2019**, 19, 242-250	19.4	17
119	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	3.6	1

118	Molecular Modeling Approach to Determine the Flory-Huggins Interaction Parameter for Polymer Miscibility Analysis. *ChemPhysChem*, **2018**, 19, 1655-1664	3.2	9
117	Detecting the functional complexities between high-density lipoprotein mimetics. *Biomaterials*, **2018**, 170, 58-69	15.6	12
116	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	15.6	1
115	Origin and Control of Polyacrylonitrile Alignments on Carbon Nanotubes and Graphene Nanoribbons. *Advanced Functional Materials*, **2018**, 28, 1706970	15.6	15
114	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	3.8	13
113	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	13	14
112	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	2.6	2
111	Density Functional Theory - Machine Learning Approach to Analyze the Bandgap of Elemental Halide Perovskites and Ruddlesden-Popper Phases. *ChemPhysChem*, **2018**, 19, 2559-2565	3.2	15
110	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	27
109	Electrochemical Properties of Boron-Doped Fullerene Derivatives for Lithium-Ion Battery Applications. *ChemPhysChem*, **2018**, 19, 753-758	3.2	24
108	Dissipative particle dynamics simulation of multicompartment micelle nanoreactor with channel for reactants.. *RSC Advances*, **2018**, 8, 37866-37871	3.7	2
107	Application of DFT-based machine learning for developing molecular electrode materials in Li-ion batteries.. *RSC Advances*, **2018**, 8, 39414-39420	3.7	49
106	Structural Tunability of Multicompartment Micelles as a Function of Lipophilic-Fluorophilic Block Length Ratio. *Journal of Physical Chemistry B*, **2018**, 122, 12164-12172	3.4	4
105	Cytoprotective Self-assembled RGD Peptide Nanofilms for Surface Modification of Viable Mesenchymal Stem Cells. *Chemistry of Materials*, **2017**, 29, 2055-2065	9.6	41
104	Systematic Molecular Design of Ketone Derivatives of Aromatic Molecules for Lithium-Ion Batteries: First-Principles DFT Modeling. *ChemSusChem*, **2017**, 10, 1584-1591	8.3	32
103	Structure and hydrophilicity of azo-dye-derived rotaxane: density functional theory approach. *Coloration Technology*, **2017**, 133, 382-390	2	1
102	Enhanced Selectivity for CO Adsorption on Mesoporous Silica with Alkali Metal Halide Due to Electrostatic Field: A Molecular Simulation Approach. *ACS Applied Materials & Interfaces*, **2017**, 9, 31683-31690	9.5	9
101	Self-polymerized dopamine as an organic cathode for Li- and Na-ion batteries. *Energy and Environmental Science*, **2017**, 10, 205-215	35.4	181

100	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	3.2	2
99	Collagen intrafibrillar mineralization as a result of the balance between osmotic equilibrium and electroneutrality. *Nature Materials*, **2017**, 16, 370-378	27	148
98	Dispersant-free dyeing of poly(lactic acid) fabric with temporarily solubilised disperse dyes from azopyridone derivatives. *Coloration Technology*, **2016**, 132, 361-367	2	1
97	Synthesis of temporarily solubilised azo disperse dyes containing a □sulphatoethylsulphonyl group and dispersant-free dyeing of polyethylene terephthalate fabric. *Coloration Technology*, **2016**, 132, 368-375	2	3
96	Interactions of Pt nanoparticles with molecular components in polymer electrolyte membrane fuel cells: multi-scale modeling approach. *RSC Advances*, **2016**, 6, 69670-69676	3.7	24
95	Activating "Invisible" Glue: Using Electron Beam for Enhancement of Interfacial Properties of Graphene-Metal Contact. *ACS Nano*, **2016**, 10, 1042-9	16.7	11
94	A mechanistic study of the interaction of water-soluble borate glass with apatite-bound heterocyclic nitrogen-containing bisphosphonates. *Acta Biomaterialia*, **2016**, 31, 339-347	10.8	5
93	Investigation of the effect of erythrosine B on amyloid beta peptide using molecular modeling. *Journal of Molecular Modeling*, **2016**, 22, 92	2	12
92	The effects of ethanol on the size-exclusion characteristics of type I dentin collagen to adhesive resin monomers. *Acta Biomaterialia*, **2016**, 33, 235-41	10.8	10
91	Dissipative particle dynamics simulation study of poly(2-oxazoline)-based multicompartment micelle nanoreactor. *Physical Chemistry Chemical Physics*, **2016**, 18, 6284-90	3.6	7
90	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, 2374-82	16.4	142
89	Investigation of ethanol infiltration into demineralized dentin collagen fibrils using molecular dynamics simulations. *Acta Biomaterialia*, **2016**, 36, 175-85	10.8	17
88	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, 20600-6	3.6	30
87	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	17.1	331
86	Molecular Dynamics Simulations of Aldol Condensation Catalyzed by Alkylamine-Functionalized Crystalline Silica Surfaces. *Journal of the American Chemical Society*, **2016**, 138, 7664-72	16.4	34
85	Investigations of the band structures of edge-defect zigzag graphene nanoribbons using density functional theory. *RSC Advances*, **2016**, 6, 39587-39594	3.7	11
84	Interaction of C□with water: first-principles modeling and environmental implications. *Environmental Science & Technology*, **2015**, 49, 1529-36	10.3	33
83	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	13	26

82	High-Density Lithium-Ion Energy Storage Utilizing the Surface Redox Reactions in Folded Graphene Films. *Chemistry of Materials*, **2015**, 27, 3291-3298	9.6	64
81	Adsorption of carboxylate on calcium carbonate (10 1□4) surface: Molecular simulation approach. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2015**, 474, 9-17	5.1	26
80	Li adsorption on a graphene□fullerene nanobud system: density functional theory approach. *RSC Advances*, **2015**, 5, 32819-32825	3.7	22
79	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	5.1	26
78	Effect of Superacidic Side Chain Structures on High Conductivity Aromatic Polymer Fuel Cell Membranes. *Macromolecules*, **2015**, 48, 7117-7126	5.5	45
77	Characterization of molecular association of poly(2-oxazoline)s-based micelles with various epoxides and diols via the Flory-Huggins theory: a molecular dynamics simulation approach. *Physical Chemistry Chemical Physics*, **2015**, 17, 29161-70	3.6	8
76	Dynamic modulation of electronic properties of graphene by localized carbon doping using focused electron beam induced deposition. *Nanoscale*, **2015**, 7, 14946-52	7.7	10
75	A first-principles study of lithium adsorption on a graphene-fullerene nanohybrid system. *ChemPhysChem*, **2015**, 16, 789-95	3.2	26
74	Effect of solvent on electrical conductivity and gas sensitivity of PEDOT: PSS polymer composite films. *Journal of Applied Polymer Science*, **2015**, 132, n/a-n/a	2.9	11
73	Localized conductive patterning via focused electron beam reduction of graphene oxide. *Applied Physics Letters*, **2015**, 106, 133109	3.4	10
72	All Solid-State Lithium Batteries Assembled with Hybrid Solid Electrolytes. *Journal of the Electrochemical Society*, **2015**, 162, A704-A710	3.9	124
71	Effect of ZnO nanoparticles morphology on UV blocking of poly(vinyl alcohol)/ZnO composite nanofibers. *Materials Letters*, **2015**, 147, 20-24	3.3	31
70	Functionalized fullerenes in water: a closer look. *Environmental Science & Technology*, **2015**, 49, 2147-55	6.3	12
69	Water distribution in dentin matrices: bound vs. unbound water. *Dental Materials*, **2015**, 31, 205-16	5.7	48
68	Effect of Uniaxial Deformation on Structure and Transport in Hydrated Nafion 117: Molecular Dynamics Simulation Study. *Materials Performance and Characterization*, **2015**, 4, 20150018	0.5	7
67	Structure Solution from Powder Diffraction of Copper 1,4-Benzenedicarboxylate. *European Journal of Inorganic Chemistry*, **2014**, 2014, 2140-2145	2.3	38
66	Controlling the physicochemical state of carbon on graphene using focused electron-beam-induced deposition. *ACS Nano*, **2014**, 8, 6805-13	16.7	17
65	A density functional theory (DFT) study of CO2 adsorption on Mg-rich minerals by enhanced charge distribution. *Computational Materials Science*, **2014**, 95, 181-186	3.2	25

64	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	3.8	58
63	Li adsorption on a Fullerene□Single wall carbon nanotube hybrid system: Density functional theory approach. *Current Applied Physics*, **2014**, 14, 1748-1754	2.6	16
62	The importance of size-exclusion characteristics of type I collagen in bonding to dentin matrices. *Acta Biomaterialia*, **2013**, 9, 9522-8	10.8	45
61	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	3.4	8
60	Adsorption of □d-glucose and cellobiose on kaolinite surfaces: Density functional theory (DFT) approach. *Applied Clay Science*, **2013**, 71, 73-81	5.2	58
59	Polymer electrolyte membranes based on poly(arylene ether sulfone) with pendant perfluorosulfonic acid. *Polymer Chemistry*, **2013**, 4, 272-281	4.9	56
58	Multi-Scale First-Principles Modeling of Three-Phase System of Polymer Electrolyte Membrane Fuel Cell. *ECS Transactions*, **2013**, 50, 155-160	1	1
57	Deswelling Mechanisms of Surface-Grafted Poly(NIPAAm) Brush: Molecular Dynamics Simulation Approach. *Journal of Physical Chemistry C*, **2012**, 116, 15974-15985	3.8	27
56	Magnetism in dopant-free ZnO nanoplates. *Nano Letters*, **2012**, 12, 576-81	11.5	59
55	Influence of SWNTs on the Preferential Alignment of Molecular Moieties in PVA Fibers. *Macromolecular Chemistry and Physics*, **2012**, 213, 617-626	2.6	12
54	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	1.9	10
53	Mechanism of Li adsorption on carbon nanotube-fullerene hybrid system: a first-principles study. *ACS Applied Materials & Interfaces*, **2011**, 3, 1186-94	9.5	26
52	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	1.7	7
51	Aromatic Ionomers with Highly Acidic Sulfonate Groups: Acidity, Hydration, and Proton Conductivity. *Macromolecules*, **2011**, 44, 8458-8469	5.5	83
50	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	3.8	21
49	First-principles study of Li adsorption in a carbon nanotube-fullerene hybrid system. *Carbon*, **2011**, 49, 286-293	10.4	45
48	Effect of temperature on structure and water transport of hydrated sulfonated poly(ether ether ketone): A molecular dynamics simulation approach. *Journal of Renewable and Sustainable Energy*, **2011**, 3, 043111	2.5	23
47	Stability of water-stable C60 clusters to OH radical oxidation and hydrated electron reduction. *Environmental Science & Technology*, **2010**, 44, 3786-92	10.3	27

46	Interfacial reactions of ozone with surfactant protein B in a model lung surfactant system. *Journal of the American Chemical Society*, **2010**, 132, 2254-63	16.4	44
45	Distribution and Diffusion of Water in Model Epoxy Molding Compound: Molecular Dynamics Simulation Approach. *IEEE Transactions on Advanced Packaging*, **2010**, 33, 333-339		20
44	Sponge Behaviors of Functionalized Few-Walled Carbon Nanotubes. *Journal of Physical Chemistry C*, **2010**, 114, 14868-14875	3.8	6
43	Structural and Electronic Properties of Sulfuric Acid-Doped Single-Walled Carbon Nanotube. *Journal of Computational and Theoretical Nanoscience*, **2010**, 7, 232-236	0.3	3
42	"Organic aqua regia"--powerful liquids for dissolving noble metals. *Angewandte Chemie - International Edition*, **2010**, 49, 7929-32	16.4	53
41	Molecular dynamics simulation study of P (VP-co-HEMA) hydrogels: effect of water content on equilibrium structures and mechanical properties. *Biomaterials*, **2009**, 30, 6130-41	15.6	61
40	Free energy barrier for molecular motions in bistable [2]rotaxane molecular electronic devices. *Journal of Physical Chemistry A*, **2009**, 113, 2136-43	2.8	38
39	Effect of monomeric sequence on mechanical properties of P(VP-co-HEMA) hydrogels at low hydration. *Journal of Physical Chemistry B*, **2009**, 113, 6604-12	3.4	27
38	Sodium Diffusion through Aluminum-Doped Zeolite BEA System: Effect of Water Solvation. *Journal of Physical Chemistry C*, **2009**, 113, 819-826	3.8	7
37	A hydrogen storage nanotank: lithium-organic pillared graphite. *Chemical Communications*, **2009**, 5427-9	5.8	16
36	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, 033101	2.5	45
35	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, 3133-40	2.8	77
34	Charge transport through polyene self-assembled monolayers from multiscale computer simulations. *Journal of Physical Chemistry B*, **2008**, 112, 14888-97	3.4	10
33	Mechanical and Transport Properties of the Poly(ethylene oxide)-Poly(acrylic acid) Double Network Hydrogel from Molecular Dynamic Simulations. *Journal of Physical Chemistry B*, **2007**, 111, 14440-14440	3.4	27
32	Structures and Transport Properties of Hydrated Water-Soluble Dendrimer-Grafted Polymer Membranes for Application to Polymer Electrolyte Membrane Fuel Cells: Classical Molecular Dynamics Approach. *Journal of Physical Chemistry C*, **2007**, 111, 2759-2769	3.8	47
31	Mechanical and transport properties of the poly(ethylene oxide)-poly(acrylic acid) double network hydrogel from molecular dynamic simulations. *Journal of Physical Chemistry B*, **2007**, 111, 1729-37	3.4	121
30	Multi-paradigm multi-scale simulations for fuel cell catalysts and membranes. *Molecular Simulation*, **2006**, 32, 251-268	2	105
29	Possible performance improvement in [2]catenane molecular electronic switches. *Applied Physics Letters*, **2006**, 88, 163112	3.4	8

28	Structures and properties of Newton black films characterized using molecular dynamics simulations. *Journal of Physical Chemistry B*, **2006**, 110, 7992-8001	3.4	91
27	Molecular dynamics simulation study on a monolayer of half [2]rotaxane self-assembled on Au(111). *Journal of the American Chemical Society*, **2005**, 127, 4959-64	16.4	43
26	Nanophase segregation and water dynamics in the dendrion diblock copolymer formed from the Fréchet polyaryl ethereal dendrimer and linear PTFE. *Journal of Physical Chemistry B*, **2005**, 109, 10154-67	3.4	55
25	Conformations and charge transport characteristics of biphenyldithiol self-assembled-monolayer molecular electronic devices: a multiscale computational study. *Journal of Chemical Physics*, **2005**, 122, 244703	3.9	41
24	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, 1563-75	16.4	185
23	Molecular dynamics simulation of amphiphilic bistable [2]rotaxane langmuir monolayers at the air/water interface. *Journal of the American Chemical Society*, **2005**, 127, 14804-16	16.4	90
22	First-principles study of the switching mechanism of [2]catenane molecular electronic devices. *Physical Review Letters*, **2005**, 94, 156801	7.4	67
21	Effect of monomeric sequence on nanostructure and water dynamics in Nafion 117. *Solid State Ionics*, **2004**, 175, 805-808	3.3	40
20	Nanophase-Segregation and Transport in Nafion 117 from Molecular Dynamics Simulations: Effect of Monomeric Sequence. *Journal of Physical Chemistry B*, **2004**, 108, 3149-3157	3.4	375
19	Thermodynamic Stability of Zimmerman Self-Assembled Dendritic Supramolecules from Atomistic Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2004**, 108, 10041-10052	3.4	11
18	Density functional theory studies of the [2]rotaxane component of the Stoddart-heath molecular switch. *Journal of the American Chemical Society*, **2004**, 126, 12636-45	16.4	66
17	Molecular Dynamics Study of a Surfactant-Mediated Decane−Water Interface: Effect of Molecular Architecture of Alkyl Benzene Sulfonate. *Journal of Physical Chemistry B*, **2004**, 108, 12130-12140	3.4	187
16	The Source of Helicity in Perfluorinated N-Alkanes. *Macromolecules*, **2003**, 36, 5331-5341	5.5	97
15	Effect of cyclic chain architecture on properties of dilute solutions of polyethylene from molecular dynamics simulations. *Journal of Chemical Physics*, **2003**, 119, 1843-1854	3.9	38
14	Off-lattice Monte Carlo simulation of hyperbranched polymers, 1 Polycondensation of AB2 type monomers. *Macromolecular Theory and Simulations*, **2000**, 9, 188-195	1.5	10
13	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	2.6	4
12	Phase transformation of poly(trimethylene terephthalate) in crystalline state: An atomistic modeling approach. *Fibers and Polymers*, **2000**, 1, 18-24	2	10
11	Monte Carlo simulation of the order−disorder transition of a symmetric cyclic diblock copolymer system. *Journal of Chemical Physics*, **1999**, 111, 1712-1720	3.9	44

10	Analysis of the mechanical behavior of poly(trimethylene terephthalate) in an amorphous state under uniaxial extension□compression condition through atomistic modeling. *Journal of Chemical Physics*, **1999**, 110, 7524-7532	3.9	29
9	Yielding and plastic behaviour of amorphous atactic poly(oxypropylene) under uniaxial compression: an atomistic modeling approach. *Polymer*, **1999**, 40, 919-925	3.9	5
8	Analysis of the mechanical behavior of amorphous atactic poly(oxypropylene) by atomistic modeling. *Macromolecular Theory and Simulations*, **1999**, 8, 1-9	1.5	12
7	Effects of Ester Interchange Reactions on the Phase Behavior of an Immiscible Polyester Blend:´ Monte Carlo Simulation. *Macromolecules*, **1999**, 32, 1679-1685	5.5	16
6	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	2.6	13
5	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	2.6	31
4	Covalent organic frameworks: Design and applications in electrochemical energy storage devices. *Informa□□Materi□y*,	23.1	2
3	Unveiled Correlations between Electron Affinity and Solvation in Redox Potential of Quinone-Based Sodium-Ion Batteries. *SSRN Electronic Journal*,	1	1
2	Ce(III)-Based Coordination-Complex-Based Efficient Radical Scavenger for Exceptional Durability Enhancement of Polymer Application in Proton-Exchange Membrane Fuel Cells and Organic Photovoltaics. *Advanced Energy and Sustainability Research*,2200011	1.6	0
1	Tailor-Made Charged Catechol-Based Polymeric Ligands to Build Robust Fuel Cells Containing Antioxidative Nanoparticles. *Advanced Electronic Materials*,2200171	6.4	0