# Jim Pfaendtner

## List of Publications by Year in Descending Order



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| 119 papers | 3,264 citations | 31 h-index | 52 g-index |
| 139 ext. papers | 3,866 ext. citations | 5.4 avg, IF | 5.92 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 119 | Membrane Structure of Aquaporin Observed with Combined Experimental and Theoretical Sum Frequency Generation Spectroscopy. *Langmuir*, **2021**, 37, 13452-13459 | 4 | 1 |
| 118 | Substitution of distal and active site residues reduces product inhibition of E1 from Acidothermus Cellulolyticus.. *Protein Engineering, Design and Selection*, **2021**, 34, | 1.9 | 1 |
| 117 | Direct Evidence for Aligned Binding of Cellulase Enzymes to Cellulose Surfaces. *Journal of Physical Chemistry Letters*, **2021**, 12, 10684-10688 | 6.4 | 0 |
| 116 | Probing the thermodynamics and kinetics of ethylene carbonate reduction at the electrode-electrolyte interface with molecular simulations. *Journal of Chemical Physics*, **2021**, 155, 204703 | 3.9 | 1 |
| 115 | Analyzing the Long Time-Scale Dynamics of Uremic Toxins Bound to Sudlow Site II in Human Serum Albumin. *Journal of Physical Chemistry B*, **2021**, 125, 2910-2920 | 3.4 | 1 |
| 114 | Ion-dependent protein-surface interactions from intrinsic solvent response. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118, | 11.5 | 5 |
| 113 | Data Science in Chemical Engineering: Applications to Molecular Science. *Annual Review of Chemical and Biomolecular Engineering*, **2021**, 12, 15-37 | 8.9 | 2 |
| 112 | Formulation and Efficacy of Catalase-Loaded Nanoparticles for the Treatment of Neonatal Hypoxic-Ischemic Encephalopathy. *Pharmaceutics*, **2021**, 13, | 6.4 | 3 |
| 111 | Quantifying the Dynamics of Protein Self-Organization Using Deep Learning Analysis of Atomic Force Microscopy Data. *Nano Letters*, **2021**, 21, 158-165 | 11.5 | 7 |
| 110 | Attention-based generative models for molecular design. *Chemical Science*, **2021**, 12, 8362-8372 | 9.4 | 6 |
| 109 | Efficient Sampling of High-Dimensional Free Energy Landscapes: A Review of Parallel Bias Metadynamics. *Molecular Modeling and Simulation*, **2021**, 123-141 | | |
| 108 | Effect of Fluoroethylene Carbonate Additives on the Initial Formation of the Solid Electrolyte Interphase on an Oxygen-Functionalized Graphitic Anode in Lithium-Ion Batteries. *ACS Applied Materials & Interfaces*, **2021**, 13, 8169-8180 | 9.5 | 6 |
| 107 | Ice-nucleating proteins are activated by low temperatures to control the structure of interfacial water. *Nature Communications*, **2021**, 12, 1183 | 17.4 | 8 |
| 106 | Deconstruction of high-density polyethylene into liquid hydrocarbon fuels and lubricants by hydrogenolysis over Ru catalyst. *Chem Catalysis*, **2021**, 1, 437-455 | | 22 |
| 105 | Effect of graphitic anode surface functionalization on the structure and dynamics of electrolytes at the interface. *Journal of Chemical Physics*, **2021**, 155, 134702 | 3.9 | 0 |
| 104 | // Virtual Special Issue on Machine Learning in Physical Chemistry. *Journal of Physical Chemistry B*, **2020**, 124, 9767-9772 | 3.4 | 2 |
| 103 | // Virtual Special Issue on Machine Learning in Physical Chemistry. *Journal of Physical Chemistry A*, **2020**, 124, 9113-9118 | 2.8 | 1 |

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| 102 | The Journal of Physical Chemistry A/B/C Virtual Special Issue on Machine Learning in Physical Chemistry. *Journal of Physical Chemistry C*, **2020**, 124, 24033-24038 | 3.8 | 1 |
| 101 | Trimethylation of the R5 Silica-Precipitating Peptide Increases Silica Particle Size by Redirecting Orthosilicate Binding. *ChemBioChem*, **2020**, 21, 3208-3211 | 3.8 | 2 |
| 100 | Sequence-Structure-Binding Relationships Reveal Adhesion Behavior of the Car9 Solid-Binding Peptide: An Integrated Experimental and Simulation Study. *Journal of the American Chemical Society*, **2020**, 142, 2355-2363 | 16.4 | 11 |
| 99 | Elucidating the Molecular Interactions between Uremic Toxins and the Sudlow II Binding Site of Human Serum Albumin. *Journal of Physical Chemistry B*, **2020**, 124, 3922-3930 | 3.4 | 2 |
| 98 | Elucidating Molecular Design Principles for Charge-Alternating Peptides. *Biomacromolecules*, **2020**, 21, 435-443 | 6.9 | 5 |
| 97 | Impact of Glutamate Carboxylation in the Adsorption of the □I Domain of Osteocalcin to Hydroxyapatite and Titania. *Molecular Systems Design and Engineering*, **2020**, 5, 620-631 | 4.6 | 4 |
| 96 | Assessing the Performance of Various Stochastic Optimization Methods on Chemical Kinetic Modeling of Combustion. *Industrial & Engineering Chemistry Research*, **2020**, 59, 19212-19225 | 3.9 | 2 |
| 95 | Enhanced Activity and Stability of Acidothermus cellulolyticus Endoglucanase 1 in Ionic Liquids via Engineering Active Site Residues and Non-Native Disulfide Bridges. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 11299-11307 | 8.3 | 8 |
| 94 | Studies of Dynamic Binding of Amino Acids to TiO Nanoparticle Surfaces by Solution NMR and Molecular Dynamics Simulations. *Langmuir*, **2020**, 36, 10341-10350 | 4 | 7 |
| 93 | MARTINI-Compatible Coarse-Grained Model for the Mesoscale Simulation of Peptoids. *Journal of Physical Chemistry B*, **2020**, 124, 7745-7764 | 3.4 | 10 |
| 92 | Solvent oligomerization pathways facilitated by electrolyte additives during solid-electrolyte interphase formation. *Physical Chemistry Chemical Physics*, **2020**, 22, 21494-21503 | 3.6 | 7 |
| 91 | Continuous Molecular Representations of Ionic Liquids. *Journal of Physical Chemistry B*, **2020**, 124, 8347-8357 | 3.4 | 8 |
| 90 | Orientation and Conformation of Proteins at the Air-Water Interface Determined from Integrative Molecular Dynamics Simulations and Sum Frequency Generation Spectroscopy. *Langmuir*, **2020**, 36, 11855-11865 | 4 | 13 |
| 89 | Closing the Gap Between Modeling and Experiments in the Self-Assembly of Biomolecules at Interfaces and in Solution□*Chemistry of Materials*, **2020**, 32, 8043-8059 | 9.6 | 4 |
| 88 | Molecular recognition and specificity of biomolecules to titanium dioxide from molecular dynamics simulations. *Npj Computational Materials*, **2020**, 6, | 10.9 | 3 |
| 87 | Metadynamics to Enhance Sampling in Biomolecular Simulations. *Methods in Molecular Biology*, **2019**, 2022, 179-200 | 1.4 | 2 |
| 86 | Amphiphilic peptide binding on crystalline vs. amorphous silica from molecular dynamics simulations. *Molecular Physics*, **2019**, 117, 3642-3650 | 1.7 | 4 |
| 85 | Assessment of molecular dynamics simulations for amorphous poly(3-hexylthiophene) using neutron and X-ray scattering experiments. *Soft Matter*, **2019**, 15, 5067-5083 | 3.6 | 10 |

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| 84 | Trimethylamine -oxide-derived zwitterionic polymers: A new class of ultralow fouling bioinspired materials. *Science Advances*, **2019**, 5, eaaw9562 | 14.3 | 81 |
| 83 | Diagnosing the Impact of External Electric Fields Chemical Kinetics: Application to Toluene Oxidation and Pyrolysis. *Journal of Physical Chemistry A*, **2019**, 123, 3080-3089 | 2.8 | 7 |
| 82 | Generic Biphasic Catalytic Approach for Producing Renewable Diesel from Fatty Acids and Vegetable Oils. *ACS Catalysis*, **2019**, 9, 3753-3763 | 13.1 | 16 |
| 81 | Molecular Driving Forces in Peptide Adsorption to Metal Oxide Surfaces. *Langmuir*, **2019**, 35, 5911-5920 | 4 | 18 |
| 80 | Fantastic Liquids and Where To Find Them: Optimizations of Discrete Chemical Space. *Journal of Chemical Information and Modeling*, **2019**, 59, 2617-2625 | 6.1 | 5 |
| 79 | Combining Molecular and Spin Dynamics Simulations with Solid-State NMR: A Case Study of Amphiphilic Lysine-Leucine Repeat Peptide Aggregates. *Journal of Physical Chemistry B*, **2019**, 123, 10913-10929 | 3.4 | 1 |
| 78 | Solid-State NMR and MD Study of the Structure of the Statherin Mutant SNa15 on Mineral Surfaces. *Journal of the American Chemical Society*, **2019**, 141, 1998-2011 | 16.4 | 10 |
| 77 | Lifting the Curse of Dimensionality on Enhanced Sampling of Reaction Networks with Parallel Bias Metadynamics. *Journal of Chemical Theory and Computation*, **2018**, 14, 2516-2525 | 6.4 | 16 |
| 76 | Peptoid Backbone Flexibilility Dictates Its Interaction with Water and Surfaces: A Molecular Dynamics Investigation. *Biomacromolecules*, **2018**, 19, 1006-1015 | 6.9 | 16 |
| 75 | Statistical models are able to predict ionic liquid viscosity across a wide range of chemical functionalities and experimental conditions. *Molecular Systems Design and Engineering*, **2018**, 3, 253-263 | 4.6 | 22 |
| 74 | Density functional tight-binding and infrequent metadynamics can capture entropic effects in intramolecular hydrogen transfer reactions. *Journal of Chemical Physics*, **2018**, 148, 154101 | 3.9 | 4 |
| 73 | Design of Polyphosphate Inhibitors: A Molecular Dynamics Investigation on Polyethylene Glycol-Linked Cationic Binding Groups. *Biomacromolecules*, **2018**, 19, 1358-1367 | 6.9 | 7 |
| 72 | Essential slow degrees of freedom in protein-surface simulations: A metadynamics investigation. *Biochemical and Biophysical Research Communications*, **2018**, 498, 274-281 | 3.4 | 22 |
| 71 | Investigating the Role of Phosphorylation in the Binding of Silaffin Peptide R5 to Silica with Molecular Dynamics Simulations. *Langmuir*, **2018**, 34, 1199-1207 | 4 | 23 |
| 70 | Biasing Smarter, Not Harder, by Partitioning Collective Variables into Families in Parallel Bias Metadynamics. *Journal of Chemical Theory and Computation*, **2018**, 14, 4985-4990 | 6.4 | 14 |
| 69 | Inhibition of the Exoglucanase Cel7A by a Douglas-Fir-Condensed Tannin. *Journal of Physical Chemistry B*, **2018**, 122, 8665-8674 | 3.4 | 1 |
| 68 | IL-Net: Using Expert Knowledge to Guide the Design of Furcated Neural Networks **2018**, | | 3 |
| 67 | Ice-binding site of surface-bound type III antifreeze protein partially decoupled from water. *Physical Chemistry Chemical Physics*, **2018**, 20, 26926-26933 | 3.6 | 14 |

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| 66 | Determining energy barriers and selectivities of a multi-pathway system with infrequent metadynamics. *Journal of Chemical Physics*, **2017**, 146, 014108 | 3.9 | 11 |
| 65 | Acetylation dictates the morphology of nanophase biosilica precipitated by a 14-amino acid leucine-lysine peptide. *Journal of Peptide Science*, **2017**, 23, 141-147 | 2.1 | 9 |
| 64 | Assessing Generic Collective Variables for Determining Reaction Rates in Metadynamics Simulations. *Journal of Chemical Theory and Computation*, **2017**, 13, 968-973 | 6.4 | 16 |
| 63 | Application of machine learning to pyrolysis reaction networks: Reducing model solution time to enable process optimization. *Computers and Chemical Engineering*, **2017**, 104, 56-63 | 4 | 39 |
| 62 | Effect of an ionic liquid/air Interface on the structure and dynamics of amphiphilic peptides. *Journal of Molecular Liquids*, **2017**, 236, 404-413 | 6 | 8 |
| 61 | The Structure of the Diatom Silaffin Peptide R5 within Freestanding Two-Dimensional Biosilica Sheets. *Angewandte Chemie - International Edition*, **2017**, 56, 8277-8280 | 16.4 | 29 |
| 60 | Thiolated Lysine-Leucine Peptides Self-Assemble into Biosilica Nucleation Pits on Gold Surfaces. *Advanced Materials Interfaces*, **2017**, 4, 1700399 | 4.6 | 1 |
| 59 | Determining dominant driving forces affecting controlled protein release from polymeric nanoparticles. *Biointerphases*, **2017**, 12, 02D412 | 1.8 | 4 |
| 58 | LK peptide side chain dynamics at interfaces are independent of secondary structure. *Physical Chemistry Chemical Physics*, **2017**, 19, 28507-28511 | 3.6 | 11 |
| 57 | Redefining the Protein-Protein Interface: Coarse Graining and Combinatorics for an Improved Understanding of Amino Acid Contributions to the Protein-Protein Binding Affinity. *Langmuir*, **2017**, 33, 11511-11517 | 4 | 1 |
| 56 | Quantifying the Molecular-Scale Aqueous Response to the Mica Surface. *Journal of Physical Chemistry C*, **2017**, 121, 18496-18504 | 3.8 | 14 |
| 55 | Enhancing the Oxidation of Toluene with External Electric Fields: a Reactive Molecular Dynamics Study. *Scientific Reports*, **2017**, 7, 1710 | 4.9 | 13 |
| 54 | Mechanism of Competitive Inhibition and Destabilization of Acidothermus cellulolyticus Endoglucanase 1 by Ionic Liquids. *Journal of Physical Chemistry B*, **2017**, 121, 10793-10803 | 3.4 | 19 |
| 53 | Elucidating sequence and solvent specific design targets to protect and stabilize enzymes for biocatalysis in ionic liquids. *Physical Chemistry Chemical Physics*, **2017**, 19, 17426-17433 | 3.6 | 20 |
| 52 | Detailed Kinetic Modeling of Lignin Pyrolysis for Process Optimization. *Industrial & Engineering Chemistry Research*, **2016**, 55, 9147-9153 | 3.9 | 31 |
| 51 | Kinetics and mechanism of ionic-liquid induced protein unfolding: application to the model protein HP35. *Molecular Systems Design and Engineering*, **2016**, 1, 382-390 | 4.6 | 29 |
| 50 | Destabilization of Human Serum Albumin by Ionic Liquids Studied Using Enhanced Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2016**, 120, 12079-12087 | 3.4 | 21 |
| 49 | Ice-nucleating bacteria control the order and dynamics of interfacial water. *Science Advances*, **2016**, 2, e1501630 | 14.3 | 128 |

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| 48 | Using Molecular Simulation to Study Biocatalysis in Ionic Liquids. *Methods in Enzymology*, **2016**, 577, 419-41 | 8 | |
| 47 | Millisecond Pulsed Films Unify the Mechanisms of Cellulose Fragmentation. *Chemistry of Materials*, **2016**, 28, 3108-3114 | 9.6 | 63 |
| 46 | New Approach for Investigating Reaction Dynamics and Rates with Ab Initio Calculations. *Journal of Physical Chemistry A*, **2016**, 120, 299-305 | 2.8 | 37 |
| 45 | Data science: Accelerating innovation and discovery in chemical engineering. *AICHE Journal*, **2016**, 62, 1402-1416 | 3.6 | 44 |
| 44 | Strong Electrostatic Interactions Lead to Entropically Favorable Binding of Peptides to Charged Surfaces. *Langmuir*, **2016**, 32, 5690-701 | 4 | 31 |
| 43 | Ultrafast Reorientational Dynamics of Leucine at the Air-Water Interface. *Journal of the American Chemical Society*, **2016**, 138, 5226-9 | 16.4 | 23 |
| 42 | Lytic Polysaccharide Monooxygenases ScLPMO10B and ScLPMO10C Are Stable in Ionic Liquids As Determined by Molecular Simulations. *Journal of Physical Chemistry B*, **2016**, 120, 3863-72 | 3.4 | 15 |
| 41 | Chain Flexibility in Self-Assembled Monolayers Affects Protein Adsorption and Surface Hydration: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2016**, 120, 10423-10432 | 3.4 | 19 |
| 40 | The general AMBER force field (GAFF) can accurately predict thermodynamic and transport properties of many ionic liquids. *Journal of Physical Chemistry B*, **2015**, 119, 5882-95 | 3.4 | 185 |
| 39 | Molecular dynamics investigation of the ionic liquid/enzyme interface: application to engineering enzyme surface charge. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 670-80 | 4.2 | 43 |
| 38 | Structure Characterization and Properties of Metal-Surfactant Complexes Dispersed in Organic Solvents. *Langmuir*, **2015**, 31, 9006-16 | 4 | 10 |
| 37 | Trp-Cage Folding on Organic Surfaces. *Journal of Physical Chemistry B*, **2015**, 119, 10417-25 | 3.4 | 24 |
| 36 | Efficient Sampling of High-Dimensional Free-Energy Landscapes with Parallel Bias Metadynamics. *Journal of Chemical Theory and Computation*, **2015**, 11, 5062-7 | 6.4 | 112 |
| 35 | Solvatochromism and conformational changes in fully dissolved poly(3-alkylthiophene)s. *Langmuir*, **2015**, 31, 458-68 | 4 | 24 |
| 34 | Enhanced sampling of chemical and biochemical reactions with metadynamics. *Molecular Simulation* , **2015**, 41, 55-72 | 2 | 34 |
| 33 | Folding and insertion thermodynamics of the transmembrane WALP peptide. *Journal of Chemical Physics*, **2015**, 143, 243127 | 3.9 | 29 |
| 32 | Biomimetic Growth of Ultrathin Silica Sheets Using Artificial Amphiphilic Peptides. *Advanced Materials Interfaces*, **2015**, 2, 1500282 | 4.6 | 29 |
| 31 | Effect of Hydrophobic and Hydrophilic Surfaces on the Stability of Double-Stranded DNA. *Biomacromolecules*, **2015**, 16, 1862-9 | 6.9 | 20 |

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| 30 | Comparison of three ionic liquid-tolerant cellulases by molecular dynamics. *Biophysical Journal*, **2015**, 108, 880-892 | 2.9 | 53 |
| 29 | Fast Pyrolysis of Wood for Biofuels: Spatiotemporally Resolved Diffuse Reflectance In situ Spectroscopy of Particles. *ChemSusChem*, **2014**, 7, 765 | 8.3 | 34 |
| 28 | Ionic Liquids Can Selectively Change the Conformational Free-Energy Landscape of Sugar Rings. *Journal of Chemical Theory and Computation*, **2014**, 10, 507-10 | 6.4 | 20 |
| 27 | Diatom mimics: directing the formation of biosilica nanoparticles by controlled folding of lysine-leucine peptides. *Journal of the American Chemical Society*, **2014**, 136, 15134-7 | 16.4 | 50 |
| 26 | CarBarrinello Molecular Dynamics + Metadynamics Study of High-Temperature Methanol Oxidation Reactions Using Generic Collective Variables. *Journal of Physical Chemistry C*, **2014**, 118, 10764-10770 | 4.8 | 30 |
| 25 | Structural effects of methionine oxidation on isolated subdomains of human fibrin D and E regions. *PLoS ONE*, **2014**, 9, e86981 | 3.7 | 28 |
| 24 | Characterizing the catalyzed hydrolysis of 1,4 glycosidic bonds using density functional theory. *Journal of Physical Chemistry A*, **2013**, 117, 14200-8 | 2.8 | 19 |
| 23 | Structure, dynamics, and activity of xylanase solvated in binary mixtures of ionic liquid and water. *ACS Chemical Biology*, **2013**, 8, 1179-86 | 4.9 | 77 |
| 22 | Exhaustively sampling peptide adsorption with metadynamics. *Langmuir*, **2013**, 29, 7999-8009 | 4 | 93 |
| 21 | Free energy of solvated salt bridges: a simulation and experimental study. *Journal of Physical Chemistry B*, **2013**, 117, 7254-9 | 3.4 | 30 |
| 20 | Structural and dynamic features of Candida rugosa lipase 1 in water, octane, toluene, and ionic liquids BMIM-PF6 and BMIM-NO3. *Journal of Physical Chemistry B*, **2013**, 117, 2662-70 | 3.4 | 49 |
| 19 | Coagulopathy In Trauma Patients Is Accompanied By Oxidation Of a Methionine Residue In The E Domain Of Fibrinogen and Abnormal Fibrin Polymerization. *Blood*, **2013**, 122, 1097-1097 | 2.2 | |
| 18 | Efficient Simulation of Explicitly Solvated Proteins in the Well-Tempered Ensemble. *Journal of Chemical Theory and Computation*, **2012**, 8, 2189-92 | 6.4 | 94 |
| 17 | Key structural features of the actin filament Arp2/3 complex branch junction revealed by molecular simulation. *Journal of Molecular Biology*, **2012**, 416, 148-61 | 6.5 | 25 |
| 16 | Actin filament remodeling by actin depolymerization factor/cofilin. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 7299-304 | 11.5 | 81 |
| 15 | Structure and dynamics of the actin filament. *Journal of Molecular Biology*, **2010**, 396, 252-63 | 6.5 | 74 |
| 14 | Nucleotide-dependent conformational states of actin. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 12723-8 | 11.5 | 97 |
| 13 | Defining coarse-grained representations of large biomolecules and biomolecular complexes from elastic network models. *Biophysical Journal*, **2009**, 97, 2327-37 | 2.9 | 70 |

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| 12 | Ab initio study of acrylate polymerization reactions: methyl methacrylate and methyl acrylate propagation. *Journal of Physical Chemistry A*, **2008**, 112, 6772-82 | 2.8 | 68 |
| 11 | A systematic methodology for defining coarse-grained sites in large biomolecules. *Biophysical Journal*, **2008**, 95, 5073-83 | 2.9 | 124 |
| 10 | Systematic multiscale parameterization of heterogeneous elastic network models of proteins. *Biophysical Journal*, **2008**, 95, 4183-92 | 2.9 | 112 |
| 9 | Molecular dynamics simulation and coarse-grained analysis of the Arp2/3 complex. *Biophysical Journal*, **2008**, 95, 5324-33 | 2.9 | 18 |
| 8 | Mechanistic Modeling of Lubricant Degradation. 2. The Autoxidation of Decane and Octane. *Industrial & Engineering Chemistry Research*, **2008**, 47, 2897-2904 | 3.9 | 46 |
| 7 | Mechanistic Modeling of Lubricant Degradation. 1. Structure□Reactivity Relationships for Free-Radical Oxidation. *Industrial & Engineering Chemistry Research*, **2008**, 47, 2886-2896 | 3.9 | 46 |
| 6 | Contra-thermodynamic behavior in intermolecular hydrogen transfer of alkylperoxy radicals. *ChemPhysChem*, **2007**, 8, 1969-78 | 3.2 | 4 |
| 5 | Tribological degradation of two vegetable-based lubricants at elevated temperatures. *Journal of Synthetic Lubrication: Research, Development and Application of Synthetic Lubricants and Functional Fluids*, **2007**, 24, 167-179 | | 7 |
| 4 | The 1-D hindered rotor approximation. *Theoretical Chemistry Accounts*, **2007**, 118, 881-898 | 1.9 | 149 |
| 3 | Elucidation of structure□reactivity relationships in hindered phenols via quantum chemistry and transition state theory. *Chemical Engineering Science*, **2007**, 62, 5232-5239 | 4.4 | 16 |
| 2 | Quantum chemical investigation of low-temperature intramolecular hydrogen transfer reactions of hydrocarbons. *Journal of Physical Chemistry A*, **2006**, 110, 10863-71 | 2.8 | 54 |
| 1 | Lexicography of kinetic modeling of complex reaction networks. *AICHE Journal*, **2005**, 51, 2112-2121 | 3.6 | 82 |