# Jeffrey J Potoff

List of Publications by Year
in descending order



| 54 | 4,599 | 218662 | 168376 |
|---|---|---|---|
| papers | citations | 26 h-index | 53 g-index |

| 55 | 55 | 55 | 3417 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Accurate determination of solvation free energies of neutral organic compounds from first principles. Nature Communications, 2022, 13, 414. | 12.8 | 14 |
| 2 | py-MCMD: Python Software for Performing Hybrid Monte Carlo/Molecular Dynamics Simulations with GOMC and NAMD. Journal of Chemical Theory and Computation, 2022, 18, 4983-4994. | 5.3 | 10 |
| 3 | Update 2.70 to â€œGOMC: GPU Optimized Monte Carlo for the simulation of phase equilibria and physical properties of complex fluidsâ€• SoftwareX, 2021, 13, 100627. | 2.6 | 5 |
| 4 | Openâ€source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. AICHE Journal, 2021, 67, e17206. | 3.6 | 16 |
| 5 | Self-Assembly and Biogenesis of the Cellular Membrane are Dictated by Membrane Stretch and Composition. Journal of Physical Chemistry B, 2019, 123, 6997-7005. | 2.6 | 3 |
| 6 | Effect of fluorination on the partitioning of alcohols. Molecular Physics, 2019, 117, 3827-3839. | 1.7 | 2 |
| 7 | Prediction of phase equilibria and Gibbs free energies of transfer using molecular exchange Monte Carlo in the Gibbs ensemble. Fluid Phase Equilibria, 2019, 486, 106-118. | 2.5 | 8 |
| 8 | Histogram-Free Reweighting with Grand Canonical Monte Carlo: Post-simulation Optimization of Non-bonded Potentials for Phase Equilibria. Journal of Chemical & Engineering Data, 2019, 64, 3701-3717. | 1.9 | 5 |
| 9 | GOMC: GPU Optimized Monte Carlo for the simulation of phase equilibria and physical properties of complex fluids. SoftwareX, 2019, 9, 20-27. | 2.6 | 32 |
| 10 | Molecular exchange Monte Carlo: A generalized method for identity exchanges in grand canonical Monte Carlo simulations. Journal of Chemical Physics, 2018, 149, 072318. | 3.0 | 7 |
| 11 | Mechanism of Membrane Biogenesis. FASEB Journal, 2018, 32, 671.11. | 0.5 | 0 |
| 12 | Optimized Mie Potentials for Phase Equilibria: Application to Branched Alkanes. Journal of Chemical & Engineering Data, 2017, 62, 1806-1818. | 1.9 | 24 |
| 13 | Optimised Mie potentials for phase equilibria: application to alkynes. Molecular Physics, 2017, 115, 1378-1388. | 1.7 | 14 |
| 14 | Improving performance of GPU code using novel features of the NVIDIA kepler architecture. Concurrency Computation Practice and Experience, 2016, 28, 3586-3605. | 2.2 | 7 |
| 15 | Prediction of Radon-222 Phase Behavior by Monte Carlo Simulation. Journal of Chemical & Engineering Data, 2016, 61, 1625-1631. | 1.9 | 13 |
| 16 | The effect of fluorination on the physical properties and the free energies of hydration of 1-alcohols. Fluid Phase Equilibria, 2016, 407, 314-321. | 2.5 | 6 |
| 17 | Evaluation of Hybrid Parallel Cell List Algorithms for Monte Carlo Simulation. , 2015, , . | | 0 |
| 18 | Optimized Mie potentials for phase equilibria: Application to noble gases and their mixtures with n-alkanes. Journal of Chemical Physics, 2015, 143, 114504. | 3.0 | 43 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Parallel Monte Carlo simulation in the canonical ensemble on the graphics processing unit. International Journal of Parallel, Emergent and Distributed Systems, 2014, 29, 379-400. | 1.0 | 4 |
| 20 | Mie Potentials for Phase Equilibria: Application to Alkenes. Journal of Chemical & Engineering Data, 2014, 59, 3144-3150. | 1.9 | 30 |
| 21 | GPU-accelerated Gibbs ensemble Monte Carlo simulations of Lennard-Jonesium. Computer Physics Communications, 2013, 184, 2662-2669. | 7.5 | 27 |
| 22 | Biomolecular Simulations with the Transferable Potentials for Phase Equilibria: Extension to Phospholipids. Journal of Physical Chemistry B, 2013, 117, 9910-9921. | 2.6 | 14 |
| 23 | Study on Interfacial Interaction between Polymer and Nanoparticle in a Nanocoating Matrix: A MARTINI Coarse-Graining Method. Industrial & Engineering Chemistry Research, 2013, 52, 73-82. | 3.7 | 22 |
| 24 | Prediction of 1-octanolâ€“water and airâ€“water partition coefficients for nitro-aromatic compounds from molecular dynamics simulations. Physical Chemistry Chemical Physics, 2013, 15, 6467. | 2.8 | 24 |
| 25 | Monte Carlo predictions of phase equilibria and structure for dimethyl ether + sulfur dioxide and dimethyl ether + carbon dioxide. Journal of Chemical Physics, 2012, 136, 044514. | 3.0 | 9 |
| 26 | Direct calculation of 1-octanolâ€“water partition coefficients from adaptive biasing force molecular dynamics simulations. Journal of Chemical Physics, 2012, 137, 014502. | 3.0 | 44 |
| 27 | Computational prediction of ionic liquid 1-octanol/water partition coefficients. Physical Chemistry Chemical Physics, 2012, 14, 4339. | 2.8 | 28 |
| 28 | Membraneâ€directed molecular assembly of the neuronal SNARE complex. Journal of Cellular and Molecular Medicine, 2011, 15, 31-37. | 3.6 | 29 |
| 29 | Development of an Optimized Intermolecular Potential for Sulfur Dioxide. Journal of Physical Chemistry B, 2011, 115, 4949-4954. | 2.6 | 65 |
| 30 | Ca<sup>2+</sup> Bridging of Apposed Phospholipid Bilayers. Journal of Physical Chemistry B, 2010, 114, 13249-13254. | 2.6 | 29 |
| 31 | Effect of torsional potential on the predicted phase behavior of n-alkanes. Fluid Phase Equilibria, 2009, 279, 100-104. | 2.5 | 10 |
| 32 | Extension of the Transferable Potentials for Phase Equilibria Force Field to Dimethylmethyl Phosphonate, Sarin, and Soman. Journal of Physical Chemistry B, 2009, 113, 10292-10297. | 2.6 | 37 |
| 33 | All-Atom Force Field for the Prediction of Vaporâ^'Liquid Equilibria and Interfacial Properties of HFA134a. Journal of Physical Chemistry B, 2009, 113, 178-187. | 2.6 | 42 |
| 34 | Mie Potentials for Phase Equilibria Calculations: Application to Alkanes and Perfluoroalkanes. Journal of Physical Chemistry B, 2009, 113, 14725-14731. | 2.6 | 110 |
| 35 | Ca<sup>2+</sup>â€“dimethylphosphate complex formation: Providing insight into Ca<sup>2+</sup>â€mediated local dehydration and membrane fusion in cells. Cell Biology International, 2008, 32, 361-366. | 3.0 | 40 |
| 36 | Development of the TraPPE-UA force field for ethylene oxide. Fluid Phase Equilibria, 2008, 274, 44-49. | 2.5 | 30 |

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|---|---|---|---|
| 37 | Effect of partial charge parameterization on the phase equilibria of dimethyl ether. Molecular Simulation, 2007, 33, 769-776. | 2.0 | 20 |
| 38 | Vaporâ˜'Liquid Equilibria of Diethylamine + Methanol, Diethylamine + Acetone and Diethylamine + Acetonitrile:â€‰ Predictions of Atomistic Computer Simulations. Journal of Physical Chemistry C, 2007, 111, 1451-1458. | 3.1 | 2 |
| 39 | Application of TraPPE-UA force field for determination of vaporâ€"liquid equilibria of carboxylate esters. Fluid Phase Equilibria, 2006, 240, 46-55. | 2.5 | 51 |
| 40 | Monte Carlo predictions for the phase behavior of H2 S+n-alkane, H2 S+CO2, CO2+CH4 and H2 S+CO2+CH4 mixtures. Fluid Phase Equilibria, 2006, 246, 71-78. | 2.5 | 24 |
| 41 | Effect of quadrupole moment on the phase behavior of binary mixtures containing ethene. Fluid Phase Equilibria, 2005, 234, 144-150. | 2.5 | 33 |
| 42 | Molecular Modeling of Phase Behavior and Microstructure of Acetoneâ˜'Chloroformâ˜'Methanol Binary Mixtures. Journal of Physical Chemistry B, 2005, 109, 19463-19473. | 2.6 | 67 |
| 43 | Transferable Potentials for Phase Equilibria. 8. United-Atom Description for Thiols, Sulfides, Disulfides, and Thiophene. Journal of Physical Chemistry B, 2005, 109, 24100-24107. | 2.6 | 112 |
| 44 | Effect of partial charge parametrization on the fluid phase behavior of hydrogen sulfide. Journal of Chemical Physics, 2005, 123, 124505. | 3.0 | 69 |
| 45 | Transferable Potentials for Phase Equilibria. 6. United-Atom Description for Ethers, Glycols, Ketones, and Aldehydes. Journal of Physical Chemistry B, 2004, 108, 17596-17605. | 2.6 | 410 |
| 46 | An Improved Force Field for the Prediction of the Vaporâ˜'Liquid Equilibria for Carboxylic Acids. Journal of Physical Chemistry B, 2004, 108, 14130-14136. | 2.6 | 82 |
| 47 | Vaporâ˜'Liquid Phase Equilibria for Linear and Branched Alkane Monolayers Physisorbed on Au(111). Langmuir, 2002, 18, 6088-6095. | 3.5 | 17 |
| 48 | Monte Carlo Calculations for Alcohols and Their Mixtures with Alkanes. Transferable Potentials for Phase Equilibria. 5. United-Atom Description of Primary, Secondary, and Tertiary Alcohols. Journal of Physical Chemistry B, 2001, 105, 3093-3104. | 2.6 | 730 |
| 49 | Monte Carlo calculations for the phase equilibria of alkanes, alcohols, water, and their mixtures. Fluid Phase Equilibria, 2001, 183-184, 301-309. | 2.5 | 44 |
| 50 | Vaporâ€"liquid equilibria of mixtures containing alkanes, carbon dioxide, and nitrogen. AICHE Journal, 2001, 47, 1676-1682. | 3.6 | 1,560 |
| 51 | Effect of Branching on the Fluid Phase Behavior of Alkane Monolayers. Physical Review Letters, 2000, 85, 3460-3463. | 7.8 | 15 |
| 52 | Adiabatic Nuclear and Electronic Sampling Monte Carlo Simulations in the Gibbs Ensemble:Â Application to Polarizable Force Fields for Water. Journal of Physical Chemistry B, 2000, 104, 2378-2390. | 2.6 | 68 |
| 53 | Surface tension of the three-dimensional Lennard-Jones fluid from histogram-reweighting Monte Carlo simulations. Journal of Chemical Physics, 2000, 112, 6411-6415. | 3.0 | 144 |
| 54 | Critical point and phase behavior of the pure fluid and a Lennard-Jones mixture. Journal of Chemical Physics, 1998, 109, 10914-10920. | 3.0 | 347 |