Ahmadreza Rahbari

List of Publications by Citations

16 papers	195 citations	10 h-index	13 g-index
16 ext. papers	269 ext. citations	3.4 avg, IF	3.32 L-index

#	Paper	IF	Citations
16	Efficient Application of Continuous Fractional Component Monte Carlo in the Reaction Ensemble. *Journal of Chemical Theory and Computation*, **2017**, 13, 4452-4466	6.4	23
15	Combined Steam Reforming of Methane and Formic Acid To Produce Syngas with an Adjustable H:CO Ratio. *Industrial & Engineering Chemistry Research*, **2018**, 57, 10663-10674	3.9	20
14	Computation of partial molar properties using continuous fractional component Monte Carlo. *Molecular Physics*, **2018**, 116, 3331-3344	1.7	19
13	Computation of thermodynamic properties in the continuous fractional component Monte Carlo Gibbs ensemble. *Molecular Simulation*, **2017**, 43, 189-195	2	17
12	Adsorption equilibrium of nitrogen dioxide in porous materials. *Physical Chemistry Chemical Physics*, **2018**, 20, 4189-4199	3.6	17
11	Solubility of Water in Hydrogen at High Pressures: A Molecular Simulation Study. *Journal of Chemical & Engineering Data*, **2019**, 64, 4103-4115	2.8	16
10	Brick-CFCMC: Open Source Software for Monte Carlo Simulations of Phase and Reaction Equilibria Using the Continuous Fractional Component Method. *Journal of Chemical Information and Modeling*, **2020**, 60, 2678-2682	6.1	14
9	Recent advances in the continuous fractional component Monte Carlo methodology. *Molecular Simulation*, **2021**, 47, 804-823	2	14
8	Chemical potentials of water, methanol, carbon dioxide and hydrogen sulphide at low temperatures using continuous fractional component Gibbs ensemble Monte Carlo. *Molecular Simulation*, **2018**, 44, 405-414	2	13
7	Improving the accuracy of computing chemical potentials in CFCMC simulations. *Molecular Physics*, **2019**, 117, 3493-3508	1.7	10
6	Multiple linear regression and thermodynamic fluctuations are equivalent for computing thermodynamic derivatives from molecular simulation. *Fluid Phase Equilibria*, **2020**, 523, 112785	2.5	10
5	Effect of truncating electrostatic interactions on predicting thermodynamic properties of water–methanol systems. *Molecular Simulation*, **2019**, 45, 336-350	2	10
4	Multiple Free Energy Calculations from Single State Point Continuous Fractional Component Monte Carlo Simulation Using Umbrella Sampling. *Journal of Chemical Theory and Computation*, **2020**, 16, 1757-1767	6.4	6
3	Effect of Water Content on Thermodynamic Properties of Compressed Hydrogen. *Journal of Chemical & Engineering Data*, **2021**, 66, 2071-2087	2.8	4
2	New Features of the Open Source Monte Carlo Software Brick-CFCMC: Thermodynamic Integration and Hybrid Trial Moves. *Journal of Chemical Information and Modeling*, **2021**, 61, 3752-3757	6.1	2
1	Electro-osmotic Drag and Thermodynamic Properties of Water in Hydrated Nafion Membranes from Molecular Dynamics.. *Journal of Physical Chemistry C*, **2022**, 126, 8121-8133	3.8	0