Othon Moultos

List of Publications by Citations

65 papers	1,166 citations	22 h-index	31 g-index
67 ext. papers	1,627 ext. citations	4.3 avg, IF	5.24 L-index

#	Paper	IF	Citations
65	Self-diffusion coefficient of bulk and confined water: a critical review of classical molecular simulation studies. *Molecular Simulation*, **2019**, 45, 425-453	2	69
64	Finite-Size Effects of Binary Mutual Diffusion Coefficients from Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2018**, 14, 2667-2677	6.4	68
63	Atomistic molecular dynamics simulations of CO□diffusivity in H□O for a wide range of temperatures and pressures. *Journal of Physical Chemistry B*, **2014**, 118, 5532-41	3.4	63
62	System-size corrections for self-diffusion coefficients calculated from molecular dynamics simulations: The case of CO2, n-alkanes, and poly(ethylene glycol) dimethyl ethers. *Journal of Chemical Physics*, **2016**, 145, 074109	3.9	60
61	Thermodynamic and Transport Properties of H2O + NaCl from Polarizable Force Fields. *Journal of Chemical Theory and Computation*, **2015**, 11, 3802-10	6.4	49
60	Molecular simulation of thermodynamic and transport properties for the H2O+NaCl system. *Journal of Chemical Physics*, **2014**, 141, 234507	3.9	49
59	Structural, Thermodynamic, and Transport Properties of Aqueous Reline and Ethaline Solutions from Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2019**, 123, 11014-11025	3.4	41
58	Atomistic Molecular Dynamics Simulations of Carbon Dioxide Diffusivity in n-Hexane, n-Decane, n-Hexadecane, Cyclohexane, and Squalane. *Journal of Physical Chemistry B*, **2016**, 120, 12890-12900	3.4	39
57	Computing solubility parameters of deep eutectic solvents from Molecular Dynamics simulations. *Fluid Phase Equilibria*, **2019**, 497, 10-18	2.5	33
56	OCTP: A Tool for On-the-Fly Calculation of Transport Properties of Fluids with the Order- n Algorithm in LAMMPS. *Journal of Chemical Information and Modeling*, **2019**, 59, 1290-1294	6.1	32
55	Self-diffusion coefficients of the binary (H 2 O + CO 2) mixture at high temperatures and pressures. *Journal of Chemical Thermodynamics*, **2016**, 93, 424-429	2.9	30
54	Brownian dynamics simulations on the self-assembly behavior of AB hybrid dendritic-star copolymers. *Langmuir*, **2011**, 27, 835-42	4	30
53	Molecular dynamics simulations of the diffusion coefficients of light n-alkanes in water over a wide range of temperature and pressure. *Fluid Phase Equilibria*, **2016**, 407, 236-242	2.5	28
52	Hydrogen-Bonding Polarizable Intermolecular Potential Model for Water. *Journal of Physical Chemistry B*, **2016**, 120, 12358-12370	3.4	28
51	On the transferability of ion parameters to the TIP4P/2005 water model using molecular dynamics simulations. *Journal of Chemical Physics*, **2020**, 152, 024501	3.9	28
50	Atomistic molecular dynamics simulations of H2O diffusivity in liquid and supercritical CO2. *Molecular Physics*, **2015**, 113, 2805-2814	1.7	27
49	Finite-size effects of diffusion coefficients computed from molecular dynamics: a review of what we have learned so far. *Molecular Simulation*, **2021**, 47, 831-845	2	27

48	Gaussian-Charge Polarizable and Nonpolarizable Models for CO2. *Journal of Physical Chemistry B*, **2016**, 120, 984-94	3.4	25
47	In Silico Screening of Metal-Organic Frameworks for Adsorption-Driven Heat Pumps and Chillers. *ACS Applied Materials & Interfaces*, **2018**, 10, 27074-27087	9.5	25
46	Shear Viscosity Computed from the Finite-Size Effects of Self-Diffusivity in Equilibrium Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2018**, 14, 5959-5968	6.4	24
45	Predictions of water/oil interfacial tension at elevated temperatures and pressures: A molecular dynamics simulation study with biomolecular force fields. *Fluid Phase Equilibria*, **2018**, 476, 30-38	2.5	23
44	The adsorption mechanisms of organic micropollutants on high-silica zeolites causing S-shaped adsorption isotherms: An experimental and Monte Carlo simulation study. *Chemical Engineering Journal*, **2020**, 389, 123968	14.7	22
43	Preferential Adsorption in Mixed Electrolytes Confined by Charged Amorphous Silica. *Journal of Physical Chemistry C*, **2019**, 123, 16711-16720	3.8	20
42	Computation of partial molar properties using continuous fractional component Monte Carlo. *Molecular Physics*, **2018**, 116, 3331-3344	1.7	19
41	Generalized Form for Finite-Size Corrections in Mutual Diffusion Coefficients of Multicomponent Mixtures Obtained from Equilibrium Molecular Dynamics Simulation. *Journal of Chemical Theory and Computation*, **2020**, 16, 3799-3806	6.4	18
40	Solubility of Water in Hydrogen at High Pressures: A Molecular Simulation Study. *Journal of Chemical & Engineering Data*, **2019**, 64, 4103-4115	2.8	16
39	Brownian Dynamics Simulations on Self-Assembly Behavior of H-Shaped Copolymers and Terpolymers.. *Macromolecules*, **2010**, 43, 6903-6911	5.5	16
38	Prediction of Composition-Dependent Self-Diffusion Coefficients in Binary Liquid Mixtures: The Missing Link for Darken-Based Models. *Industrial & Engineering Chemistry Research*, **2018**, 57, 14784-14794	3.9	15
37	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
36	Computation of gas solubilities in choline chloride urea and choline chloride ethylene glycol deep eutectic solvents using Monte Carlo simulations. *Journal of Molecular Liquids*, **2020**, 316, 113729	6	14
35	Recent advances in the continuous fractional component Monte Carlo methodology. *Molecular Simulation*, **2021**, 47, 804-823	2	14
34	On the validity of the StokesEinstein relation for various water force fields. *Molecular Physics*, **2020**, 118, e1702729	1.7	13
33	Kirkwood-Buff Integrals Using Molecular Simulation: Estimation of Surface Effects. *Nanomaterials*, **2020**, 10,	5.4	12
32	Using clathrate hydrates for gas storage and gas-mixture separations: experimental and computational studies at multiple length scales. *Molecular Physics*, **2018**, 116, 2041-2060	1.7	12
31	Diffusivity of -, -, -cyclodextrin and the inclusion complex of -cyclodextrin: Ibuprofen in aqueous solutions; A molecular dynamics simulation study. *Fluid Phase Equilibria*, **2021**, 528, 112842	2.5	11

30	Inclusion Complexation of Organic Micropollutants with Cyclodextrin. *Journal of Physical Chemistry B*, **2020**, 124, 1218-1228	3.4	10
29	Multiple linear regression and thermodynamic fluctuations are equivalent for computing thermodynamic derivatives from molecular simulation. *Fluid Phase Equilibria*, **2020**, 523, 112785	2.5	10
28	Modeling the phase equilibria of asymmetric hydrocarbon mixtures using molecular simulation and equations of state. *AICHE Journal*, **2019**, 65, 792-803	3.6	10
27	Optimizing Nonbonded Interactions of the OPLS Force Field for Aqueous Solutions of Carbohydrates: How to Capture Both Thermodynamics and Dynamics. *Journal of Chemical Theory and Computation*, **2018**, 14, 6690-6700	6.4	10
26	Micellization Properties of Shaped, Figure-Eight-Shaped and Linked Rings Copolymers. *Macromolecules*, **2014**, 47, 5851-5859	5.5	9
25	Two-Phase Equilibrium Conditions in Nanopores. *Nanomaterials*, **2020**, 10,	5.4	9
24	The effect of hydrogen content and yield strength on the distribution of hydrogen in steel: a diffusion coupled micromechanical FEM study. *Acta Materialia*, **2021**, 209, 116799	8.4	8
23	Efficient hydrogen storage in defective graphene and its mechanical stability: A combined density functional theory and molecular dynamics simulation study. *International Journal of Hydrogen Energy*, **2021**, 46, 5485-5494	6.7	8
22	Thermal conductivity of aqueous solutions of reline, ethaline, and glyceline deep eutectic solvents; a molecular dynamics simulation study. *Molecular Physics*,e1876263	1.7	8
21	Off lattice Monte Carlo simulations of AB hybrid dendritic star copolymers. *Polymer*, **2009**, 50, 328-335	3.9	7
20	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
19	Self-Assembly Behavior of Thermoresponsive Bis-Solvophilic Linear Block Terpolymers: A Simulation Study. *Macromolecules*, **2012**, 45, 2570-2579	5.5	6
18	Thermodynamic, transport, and structural properties of hydrophobic deep eutectic solvents composed of tetraalkylammonium chloride and decanoic acid. *Journal of Chemical Physics*, **2021**, 154, 144502	3.9	6
17	Reversible Hydrogen Storage in Metal-Decorated Honeycomb Borophene Oxide. *ACS Applied Materials & Interfaces*, **2021**, 13, 43233-43240	9.5	6
16	Gibbs Ensemble Monte Carlo Simulation of Fluids in Confinement: Relation between the Differential and Integral Pressures. *Nanomaterials*, **2020**, 10,	5.4	5
15	Solubility of Carbon Dioxide, Hydrogen Sulfide, Methane, and Nitrogen in Monoethylene Glycol; Experiments and Molecular Simulation. *Journal of Chemical & Engineering Data*, **2021**, 66, 524-534	2.8	5
14	How sensitive are physical properties of choline chloride-urea mixtures to composition changes: Molecular dynamics simulations and Kirkwood-Buff theory. *Journal of Chemical Physics*, **2021**, 154, 184502	3.9	5
13	Effect of Water Content on Thermodynamic Properties of Compressed Hydrogen. *Journal of Chemical & Engineering Data*, **2021**, 66, 2071-2087	2.8	4

List of Publications

12	Entropic effects in mixed micelles formed by star/linear and star/star AB copolymers. *Journal of Polymer Science, Part B: Polymer Physics*, **2015**, 53, 442-452	2.6	3
11	Electroreduction of CO/CO to C Products: Process Modeling, Downstream Separation, System Integration, and Economic Analysis.. *Industrial & Engineering Chemistry Research*, **2021**, 60, 17862-17880	3.8	3
10	13 The Role of Molecular Thermodynamics in Developing Industrial Processes and Novel Products That Meet the Needs for a Sustainable Future. *Green Chemistry and Chemical Engineering*, **2017**, 633-660		2
9	Interfacial Properties of Hydrophobic Deep Eutectic Solvents with Water. *Journal of Physical Chemistry B*, **2021**, 125, 12303-12314	3.4	2
8	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
7	Rayleigh-Brillouin light scattering spectra of CO2 from molecular dynamics. *Journal of Chemical Physics*, **2019**, 151, 064201	3.9	1
6	Entropic effects, shape, and size of mixed micelles formed by copolymers with complex architectures. *Physical Review E*, **2015**, 92, 052601	2.4	1
5	Artificial intelligence and thermodynamics help solving arson cases. *Scientific Reports*, **2020**, 10, 20502	4.9	1
4	In Silico Screening of Zeolites for High-Pressure Hydrogen Drying. *ACS Applied Materials & Interfaces*, **2021**, 13, 8383-8394	9.5	1
3	Engineering Model for Predicting the Intradiffusion Coefficients of Hydrogen and Oxygen in Vapor, Liquid, and Supercritical Water based on Molecular Dynamics Simulations. *Journal of Chemical & Engineering Data*, **2021**, 66, 3226-3244	2.8	1
2	Vapor pressures and vapor phase compositions of choline chloride urea and choline chloride ethylene glycol deep eutectic solvents from molecular simulation. *Journal of Chemical Physics*, **2021**, 155, 114504	3.9	1
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