Philippe M Ungerer

List of Publications by Year
in descending order

52	3,268	159585 30	182427 51
papers	citations	h-index	g-index

55	55	55	2141
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular Modeling of the Volumetric and Thermodynamic Properties of Kerogen: Influence of Organic Type and Maturity. Energy & Fuels, 2015, 29, 91-105.	5.1	404
2	Optimization of the anisotropic united atoms intermolecular potential forn-alkanes. Journal of Chemical Physics, 2000, 112, 5499-5510.	3.0	270
3	Transport of Multicomponent Hydrocarbon Mixtures in Shale Organic Matter by Molecular Simulations. Journal of Physical Chemistry C, 2015, 119, 22587-22595.	3.1	166
4	Molecular Simulation of Bulk Organic Matter in Type II Shales in the Middle of the Oil Formation Window. Energy & Fuels, 2014, 28, 7457-7466.	5.1	161
5	New optimization method for intermolecular potentials: Optimization of a new anisotropic united atoms potential for olefins: Prediction of equilibrium properties. Journal of Chemical Physics, 2003, 118, 3020-3034.	3.0	142
6	Molecular simulation studies of water physisorption in zeolites. Physical Chemistry Chemical Physics, 2006, 8, 5396.	2.8	139
7	Kinetic modelling of oil cracking. Organic Geochemistry, 1988, 13, 857-868.	1.8	138
8	Molecular simulation and modelisation of methane/ethane mixtures adsorption onto a microporous molecular model of kerogen under typical reservoir conditions. Microporous and Mesoporous Materials, 2014, 197, 194-203.	4.4	135
9	A General Guidebook for the Theoretical Prediction of Physicochemical Properties of Chemicals for Regulatory Purposes. Chemical Reviews, 2015, 115, 13093-13164.	47.7	116
10	Prediction of thermodynamic derivative properties of fluids by Monte Carlo simulation. Physical Chemistry Chemical Physics, 2001, 3, 4333-4339.	2.8	110
11	Development of a transferable guestâ€“host force field for adsorption of hydrocarbons in zeolites : I. Reinvestigation of alkane adsorption in silicalite by grand canonical Monte Carlo simulation. Physical Chemistry Chemical Physics, 2003, 5, 3684-3693.	2.8	107
12	Molecular simulation of the thermophysical properties of fluids: From understanding toward quantitative predictions. Journal of Molecular Liquids, 2007, 134, 71-89.	4.9	99
13	Sensitivity of the aggregation behaviour of asphaltenes to molecular weight and structure using molecular dynamics. Molecular Simulation, 2014, 40, 115-122.	2.0	96
14	Prediction of Equilibrium Properties of Cyclic Alkanes by Monte Carlo SimulationNew Anisotropic United Atoms Intermolecular PotentialNew Transfer Bias Method. Journal of Physical Chemistry B, 2002, 106, 5483-5491.	2.6	88
15	Critical point estimation of the Lennard-Jones pure fluid and binary mixtures. Journal of Chemical Physics, 2006, 125, 054515.	3.0	83
16	Monte Carlo simulation of branched alkanes and long chain n -alkanes with anisotropic united atoms intermolecular potential. Molecular Simulation, 2002, 28, 317-336.	2.0	79
17	Development of a Transferable Guestâ"Host Force Field for Adsorption of Hydrocarbons in Zeolites. II. Prediction of Alkenes Adsorption and Alkane/Alkene Selectivity in Silicalite. Journal of Physical Chemistry B, 2004, 108, 393-398.	2.6	57
18	Prediction of thermodynamic derivative properties of natural condensate gases at high pressure by Monte Carlo simulation. Fluid Phase Equilibria, 2004, 220, 211-223.	2.5	56

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19	Optimized Intermolecular Potential for Aromatic Hydrocarbons Based on Anisotropic United Atoms. 1. Benzene. Journal of Physical Chemistry B, 2004, 108, 14109-14114.	2.6	50
20	Anisotropic United Atom Model Including the Electrostatic Interactions of Methylbenzenes. I. Thermodynamic and Structural Propertiesâ€. Journal of Physical Chemistry C, 2007, 111, 15686-15699.	3.1	50
21	Optimized Intermolecular Potential for Aromatic Hydrocarbons Based on Anisotropic United Atoms. III. Polyaromatic and Naphthenoaromatic Hydrocarbons. Journal of Physical Chemistry B, 2005, 109, 2970-2976.	2.6	48
22	Optimization of the anisotropic united atoms intermolecular potential for n-alkanes: Improvement of transport properties. Journal of Chemical Physics, 2006, 125, 044517.	3.0	44
23	Thermodynamic behavior of the CO2+SO2 mixture: Experimental and Monte Carlo simulation studies. Energy Procedia, 2009, 1, 1641-1647.	1.8	43
24	Application of Gibbs Ensemble and NPT Monte Carlo Simulation to the Development of Improved Processes for H2S-rich Gases. Molecular Simulation, 2004, 30, 631-648.	2.0	38
25	Anisotropic United Atom Model Including the Electrostatic Interactions of Benzene. Journal of Physical Chemistry B, 2007, 111, 3730-3741.	2.6	38
26	Adsorption of n-alkanes in faujasite zeolites: molecular simulation study and experimental measurements. Adsorption, 2007, 13, 439-451.	3.0	38
27	Composition Analysis and Viscosity Prediction of Complex Fuel Mixtures Using a Molecular-Based Approach. Energy & Fuels, 2012, 26, 2220-2230.	5.1	38
28	Optimized Intermolecular Potential for Aromatic Hydrocarbons Based on Anisotropic United Atoms. 2. Alkylbenzenes and Styrene. Journal of Physical Chemistry B, 2004, 108, 14115-14123.	2.6	37
29	Molecular simulation applied to fluid properties in the oil and gas industry. Molecular Simulation, 2007, 33, 287-304.	2.0	34
30	Thermodynamic Behavior of the CO₂ + NO₂/N₂O₄ Mixture: A Monte Carlo Simulation Study. Journal of Physical Chemistry B, 2008, 112, 15783-15792.	2.6	32
31	Molecular simulation of the solubility and diffusion of carbon dioxide and hydrogen sulfide in polyethylene melts. Fluid Phase Equilibria, 2007, 261, 168-175.	2.5	30
32	Thermodynamic study of binary systems containing sulphur dioxide: Measurements and molecular modelling. Fluid Phase Equilibria, 2011, 304, 21-34.	2.5	28
33	Dynamical and structural properties of benzene in supercritical water. Journal of Chemical Physics, 2004, 121, 10566-10576.	3.0	27
34	High-Throughput Calculations of Molecular Properties in the MedeA Environment: Accuracy of PM7 in Predicting Vibrational Frequencies, Ideal Gas Entropies, Heat Capacities, and Gibbs Free Energies of Organic Molecules. Journal of Chemical & Engineering Data, 2014, 59, 3136-3143.	1.9	26
35	Anisotropic United-Atoms (AUA) Potential for Alcohols. Journal of Physical Chemistry B, 2008, 112, 9853-9863.	2.6	25
36	An Anisotropic United Atoms (AUA) Potential for Thiophenes. Journal of Physical Chemistry B, 2007, 111, 4460-4466.	2.6	22

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37	Accuracy of the volumetric predictions of some important equations of state for hydrocarbons, including a modified version of the Lee-Kesler method. Fluid Phase Equilibria, 1995, 106, 81-109.	2.5	21
38	Overview of MedeA^{Â®}-GIBBS capabilities for thermodynamic property calculation and VLE behaviour description of pure compounds and mixtures: application to polar compounds generated from ligno-cellulosic biomass. Molecular Simulation, 2013, 39, 1165-1211.	2.0	21
39	Direct calculation of bubble points for alkane mixtures by molecular simulation. Molecular Physics, 2001, 99, 1423-1434.	1.7	20
40	Anisotropic United Atom Model Including the Electrostatic Interactions of Methylbenzenes. II. Transport Propertiesâ€. Journal of Physical Chemistry C, 2007, 111, 15942-15951.	3.1	20
41	Molecular simulations on volumetric properties of natural gas. Fluid Phase Equilibria, 1999, 161, 45-62.	2.5	18
42	Prediction of thermodynamic properties of heavy hydrocarbons by Monte Carlo simulation. Fluid Phase Equilibria, 2004, 224, 73-81.	2.5	18
43	Adsorption of Linear Alkanes in Zeolite Ferrierite from Molecular Simulations. Molecular Simulation, 2004, 30, 593-599.	2.0	8
44	Automatic and Systematic Atomistic Simulations in the MedeA^{Â®}Software Environment: Application to EU-REACH. Oil and Gas Science and Technology, 2015, 70, 405-417.	1.4	8
45	Compositional Modeling of Crude Oils Using C₁₀â€“C₃₆ Properties Generated by Molecular Simulation. Energy & Fuels, 2019, 33, 2967-2980.	5.1	8
46	Prediction of thermodynamic properties of heavy hydrocarbons by Monte Carlo simulation. Fluid Phase Equilibria, 2005, 228-229, 311-319.	2.5	7
47	Force Field Optimization for Organic Mercury Compounds. Journal of Physical Chemistry B, 2004, 108, 8419-8426.	2.6	6
48	Adsorption of n-Alkanes in Faujasite Zeolites: Molecular Simulation Study and Experimental Measurements. Adsorption Science and Technology, 2006, 24, 713-735.	3.2	6
49	Software Platforms for Electronic/Atomistic/Mesoscopic Modeling: Status and Perspectives. Integrating Materials and Manufacturing Innovation, 2017, 6, 92-110.	2.6	6
50	Optimized intermolecular potential for nitriles based on Anisotropic United Atoms model. Journal of Molecular Modeling, 2008, 14, 571-580.	1.8	5
51	Application of molecular simulation in the gibbs ensemble to predict liquid-vapor equilibrium curve of acetonitrile. Computer Aided Chemical Engineering, 2003, 14, 653-658.	0.5	2
52	Low-Temperature Vaporâ"Liquid Equilibria from Parallelized Molecular Dynamics Simulations. Application to 1- and 2-Methylnaphthalene. Journal of Physical Chemistry B, 2006, 110, 12083-12088.	2.6	0