Philippe M Ungerer

List of Publications by Year
in descending order

52	3,268	182225	206121
papers	citations	30 h-index	51 g-index

55	55	55	2436
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Compositional Modeling of Crude Oils Using C₁₀â€“C₃₆ Properties Generated by Molecular Simulation. Energy & Fuels, 2019, 33, 2967-2980.	2.5	8
2	Software Platforms for Electronic/Atomistic/Mesoscopic Modeling: Status and Perspectives. Integrating Materials and Manufacturing Innovation, 2017, 6, 92-110.	1.2	6
3	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
4	Transport of Multicomponent Hydrocarbon Mixtures in Shale Organic Matter by Molecular Simulations. Journal of Physical Chemistry C, 2015, 119, 22587-22595.	1.5	166
5	A General Guidebook for the Theoretical Prediction of Physicochemical Properties of Chemicals for Regulatory Purposes. Chemical Reviews, 2015, 115, 13093-13164.	23.0	116
6	Molecular Modeling of the Volumetric and Thermodynamic Properties of Kerogen: Influence of Organic Type and Maturity. Energy & Fuels, 2015, 29, 91-105.	2.5	404
7	Molecular Simulation of Bulk Organic Matter in Type II Shales in the Middle of the Oil Formation Window. Energy & Fuels, 2014, 28, 7457-7466.	2.5	161
8	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.	1.0	26
9	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.	2.2	135
10	Sensitivity of the aggregation behaviour of asphaltenes to molecular weight and structure using molecular dynamics. Molecular Simulation, 2014, 40, 115-122.	0.9	96
11	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.	0.9	21
12	Composition Analysis and Viscosity Prediction of Complex Fuel Mixtures Using a Molecular-Based Approach. Energy & Fuels, 2012, 26, 2220-2230.	2.5	38
13	Thermodynamic study of binary systems containing sulphur dioxide: Measurements and molecular modelling. Fluid Phase Equilibria, 2011, 304, 21-34.	1.4	28
14	Thermodynamic behavior of the CO2+SO2 mixture: Experimental and Monte Carlo simulation studies. Energy Procedia, 2009, 1, 1641-1647.	1.8	43
15	Optimized intermolecular potential for nitriles based on Anisotropic United Atoms model. Journal of Molecular Modeling, 2008, 14, 571-580.	0.8	5
16	Thermodynamic Behavior of the CO₂ + NO₂/N₂O₄ Mixture: A Monte Carlo Simulation Study. Journal of Physical Chemistry B, 2008, 112, 15783-15792.	1.2	32
17	Anisotropic United-Atoms (AUA) Potential for Alcohols. Journal of Physical Chemistry B, 2008, 112, 9853-9863.	1.2	25
18	Anisotropic United Atom Model Including the Electrostatic Interactions of Methylbenzenes. I. Thermodynamic and Structural Propertiesâ€. Journal of Physical Chemistry C, 2007, 111, 15686-15699.	1.5	50

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19	Anisotropic United Atom Model Including the Electrostatic Interactions of Methylbenzenes. II. Transport Propertiesâ€. Journal of Physical Chemistry C, 2007, 111, 15942-15951.	1.5	20
20	An Anisotropic United Atoms (AUA) Potential for Thiophenes. Journal of Physical Chemistry B, 2007, 111, 4460-4466.	1.2	22
21	Anisotropic United Atom Model Including the Electrostatic Interactions of Benzene. Journal of Physical Chemistry B, 2007, 111, 3730-3741.	1.2	38
22	Molecular simulation applied to fluid properties in the oil and gas industry. Molecular Simulation, 2007, 33, 287-304.	0.9	34
23	Molecular simulation of the thermophysical properties of fluids: From understanding toward quantitative predictions. Journal of Molecular Liquids, 2007, 134, 71-89.	2.3	99
24	Adsorption of n-alkanes in faujasite zeolites: molecular simulation study and experimental measurements. Adsorption, 2007, 13, 439-451.	1.4	38
25	Molecular simulation of the solubility and diffusion of carbon dioxide and hydrogen sulfide in polyethylene melts. Fluid Phase Equilibria, 2007, 261, 168-175.	1.4	30
26	Optimization of the anisotropic united atoms intermolecular potential for n-alkanes: Improvement of transport properties. Journal of Chemical Physics, 2006, 125, 044517.	1.2	44
27	Molecular simulation studies of water physisorption in zeolites. Physical Chemistry Chemical Physics, 2006, 8, 5396.	1.3	139
28	Critical point estimation of the Lennard-Jones pure fluid and binary mixtures. Journal of Chemical Physics, 2006, 125, 054515.	1.2	83
29	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.	1.2	0
30	Adsorption of n-Alkanes in Faujasite Zeolites: Molecular Simulation Study and Experimental Measurements. Adsorption Science and Technology, 2006, 24, 713-735.	1.5	6
31	Prediction of thermodynamic properties of heavy hydrocarbons by Monte Carlo simulation. Fluid Phase Equilibria, 2005, 228-229, 311-319.	1.4	7
32	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.	1.2	48
33	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.	0.9	38
34	Adsorption of Linear Alkanes in Zeolite Ferrierite from Molecular Simulations. Molecular Simulation, 2004, 30, 593-599.	0.9	8
35	Optimized Intermolecular Potential for Aromatic Hydrocarbons Based on Anisotropic United Atoms. 2. Alkylbenzenes and Styrene. Journal of Physical Chemistry B, 2004, 108, 14115-14123.	1.2	37
36	Optimized Intermolecular Potential for Aromatic Hydrocarbons Based on Anisotropic United Atoms. 1. Benzene. Journal of Physical Chemistry B, 2004, 108, 14109-14114.	1.2	50

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37	Prediction of thermodynamic properties of heavy hydrocarbons by Monte Carlo simulation. Fluid Phase Equilibria, 2004, 224, 73-81.	1.4	18
38	Prediction of thermodynamic derivative properties of natural condensate gases at high pressure by Monte Carlo simulation. Fluid Phase Equilibria, 2004, 220, 211-223.	1.4	56
39	Force Field Optimization for Organic Mercury Compounds. Journal of Physical Chemistry B, 2004, 108, 8419-8426.	1.2	6
40	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.	1.2	57
41	Dynamical and structural properties of benzene in supercritical water. Journal of Chemical Physics, 2004, 121, 10566-10576.	1.2	27
42	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.	1.3	107
43	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.	1.2	142
44	Application of molecular simulation in the gibbs ensemble to predict liquid-vapor equilibrium curve of acetonitrile. Computer Aided Chemical Engineering, 2003, 14, 653-658.	0.3	2
45	Monte Carlo simulation of branched alkanes and long chain n -alkanes with anisotropic united atoms intermolecular potential. Molecular Simulation, 2002, 28, 317-336.	0.9	79
46	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.	1.2	88
47	Direct calculation of bubble points for alkane mixtures by molecular simulation. Molecular Physics, 2001, 99, 1423-1434.	0.8	20
48	Prediction of thermodynamic derivative properties of fluids by Monte Carlo simulation. Physical Chemistry Chemical Physics, 2001, 3, 4333-4339.	1.3	110
49	Optimization of the anisotropic united atoms intermolecular potential forn-alkanes. Journal of Chemical Physics, 2000, 112, 5499-5510.	1.2	270
50	Molecular simulations on volumetric properties of natural gas. Fluid Phase Equilibria, 1999, 161, 45-62.	1.4	18
51	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.	1.4	21
52	Kinetic modelling of oil cracking. Organic Geochemistry, 1988, 13, 857-868.	0.9	138