Aziz Ghoufi

List of Publications by Year
in descending order

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148 papers	5,878 citations	71102 41 h-index	88630 70 g-index
152 all docs	152 docs citations	152 times ranked	5577 citing authors

#	Article	IF	Citations
1	Effective Separation of Hexane Isomers in the Zr-MIL-140B Metalâ€“Organic Framework Assisted by Applying Mechanical Pressure. Journal of Physical Chemistry C, 2022, 126, 2905-2911.	3.1	7
2	Interactions between methanol/toluene binary mixtures and an organic solvent nanofiltration PIM-1 membrane. Journal of Molecular Liquids, 2022, 357, 119146.	4.9	2
3	Tuning the hexane isomer separation performances of Zeolitic Imidazole Framework-8 using mechanical pressure. Journal of Chemical Physics, 2021, 154, 084702.	3.0	9
4	Dynamics of water confined in mesopores with variable surface interaction. Journal of Chemical Physics, 2021, 154, 094505.	3.0	25
5	Static dielectric permittivity of ionic liquids ultraconfined in carbon nanotubes. Nano Express, 2021, 2, 010036.	2.4	0
6	Associated molecular liquids at the graphene monolayer interface. Journal of Chemical Physics, 2021, 154, 104504.	3.0	6
7	Interfacial tension of the grapheneâ€“water solidâ€“liquid interface: how to handle the electrostatic interactions?. Molecular Physics, 2021, 119, .	1.7	2
8	Effect of the alkyl chain length on the non-ideality and the microstructure of alcohol binary mixtures. Chemical Physics Letters, 2021, 775, 138654.	2.6	3
9	Molecular Insight into the Slow Dynamics of C₄ Hydrocarbons in the Zeoliticâ€“Imidazole Framework (ZIF-8). ACS Applied Materials & Interfaces, 2021, 13, 33685-33692.	8.0	7
10	Anomalous dynamics of water at the octopeptide lanreotide surface. RSC Advances, 2020, 10, 33903-33910.	3.6	0
11	Hexane isomers separation on an isoreticular series of microporous Zr carboxylate metal organic frameworks. Journal of Materials Chemistry A, 2020, 8, 17780-17789.	10.3	15
12	Molecular Origin of the Prepeak in the Structure Factor of Alcohols. Journal of Physical Chemistry B, 2020, 124, 11501-11509.	2.6	14
13	Dynamic Heterogeneities in Liquid Mixtures Confined in Nanopores. Journal of Physical Chemistry B, 2020, 124, 3152-3162.	2.6	8
14	Tailoring the separation properties of flexible metal-organic frameworks using mechanical pressure. Nature Communications, 2020, 11, 1216.	12.8	88
15	Computational Assessment of Water Desalination Performance of Multiâ€Walled Carbon Nanotubes. Advanced Theory and Simulations, 2020, 3, 1900254.	2.8	5
16	Water nano-diffusion through the Nafion fuel cell membrane. Journal of Membrane Science, 2020, 602, 117958.	8.2	21
17	Symmetry breakings in a metal organic framework with a confined guest. Physical Review B, 2020, 101, .	3.2	10
18	Force-Field Simulations of a Hydrated Lanreotide-Based Derivative: Hydration, Dynamics, and Numerical Evidence of Self-Assembly in Dimers. ACS Omega, 2020, 5, 25423-25431.	3.5	0

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19	Force-Field Simulations of a Hydrated Lanreotide-Based Derivative: Hydration, Dynamics, and Numerical Evidence of Self-Assembly in Dimers. ACS Omega, 2020, 5, 25423-25431.	3.5	0
20	Contact angle and surface tension of water on a hexagonal boron nitride monolayer: a methodological investigation. Molecular Simulation, 2019, 45, 454-461.	2.0	20
21	Calculation of the surface tension of water: 40 years of molecular simulations. Molecular Simulation, 2019, 45, 295-303.	2.0	19
22	Single-File Diffusion of Neo-Pentane Confined in the MIL-47(V) Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2019, 123, 17360-17367.	3.1	12
23	Microstructure of nonideal methanol binary liquid mixtures. Physical Review E, 2019, 99, 062607.	2.1	20
24	Microphase separation of a miscible binary liquid mixture under confinement at the nanoscale. Npj Computational Materials, 2019, 5, .	8.7	12
25	Anomalous Dynamics of a Nanoconfined Gas in a Soft Metalâ€“Organics Framework. Journal of Physical Chemistry Letters, 2019, 10, 1698-1708.	4.6	5
26	Calculation of the interfacial tension of the graphene-water interaction by molecular simulations. Journal of Chemical Physics, 2019, 150, 014703.	3.0	26
27	Size-effects on the surface tension near the critical point: Monte Carlo simulations of the Lennard-Jones fluid. Chemical Physics Letters, 2018, 694, 60-64.	2.6	8
28	Numerical evidence of heterogeneity and nanophases in a binary liquid confined at the nanoscale. Molecular Simulation, 2018, 44, 728-735.	2.0	1
29	How Does the Surface Tension Depend on the Surface Area with Coarse-Grained Models?. Journal of Chemical Theory and Computation, 2018, 14, 2644-2651.	5.3	14
30	Nanofiltration performance of conical and hourglass nanopores. Journal of Membrane Science, 2018, 552, 336-340.	8.2	32
31	Radial-based tail methods for Monte Carlo simulations of cylindrical interfaces. Journal of Chemical Physics, 2018, 148, 094702.	3.0	2
32	The extent of the glass transition from molecular simulation revealing an overcrank effect. Journal of Computational Chemistry, 2018, 39, 255-261.	3.3	17
33	Thermal and Guest-Assisted Structural Transition in the NH2-MIL-53(Al) Metal Organic Framework: A Molecular Dynamics Simulation Investigation. Nanomaterials, 2018, 8, 531.	4.1	4
34	High Water Flux with Ions Sieving in a Desalination 2D Sub-Nanoporous Boron Nitride Material. ACS Omega, 2018, 3, 6305-6310.	3.5	28
35	Coarse-grained modeling of the oilâ€“waterâ€“surfactant interface through the local definition of the pressure tensor and interfacial tension. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	19
36	Role of MOF surface defects on the microscopic structure of MOF/polymer interfaces: A computational study of the ZIF-8/PIMs systems. Microporous and Mesoporous Materials, 2017, 254, 184-191.	4.4	30

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37	Interactions of Organics within Hydrated Selective Layer of Reverse Osmosis Desalination Membrane: A Combined Experimental and Computational Study. Environmental Science & Technology, 2017, 51, 2714-2719.	10.0	21
38	Room temperature self- and H2-broadened line parameters of carbon monoxide in the first overtone band: Theoretical and revised experimental results. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 203, 309-324.	2.3	18
39	Importance of the tail corrections on surface tension of curved liquid-vapor interfaces. Journal of Chemical Physics, 2017, 146, 084703.	3.0	11
40	Test-area surface tension calculation of the graphene-methane interface: Fluctuations and commensurability. Journal of Chemical Physics, 2017, 146, 214112.	3.0	14
41	Electrically Induced Breathing of the MIL-53(Cr) Metalâ€“Organic Framework. ACS Central Science, 2017, 3, 394-398.	11.3	102
42	Is Fineâ€€Grained Simulation Able to Propose New Polyelectrolyte Membranes?. Fuel Cells, 2016, 16, 675-681.	2.4	7
43	Can we approach the gasâ€“liquid critical point using slab simulations of two coexisting phases?. Journal of Chemical Physics, 2016, 145, 124702.	3.0	5
44	Influence of the interface on the optical activity of confined glucose films. Journal of Colloid and Interface Science, 2016, 477, 103-108.	9.4	1
45	Pressure-driven molecular dynamics simulations of water transport through a hydrophilic nanochannel. Molecular Physics, 2016, 114, 2655-2663.	1.7	30
46	Microphase Separation of Binary Liquids Confined in Cylindrical Pores. Journal of Physical Chemistry C, 2016, 120, 9245-9252.	3.1	24
47	Physics behind Water Transport through Nanoporous Boron Nitride and Graphene. Journal of Physical Chemistry Letters, 2016, 7, 3371-3376.	4.6	70
48	Ultrafast diffusion of Ionic Liquids Confined in Carbon Nanotubes. Scientific Reports, 2016, 6, 28518.	3.3	62
49	Physical Properties and Hydrogen-Bonding Network of Waterâ€“Ethanol Mixtures from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2016, 120, 793-802.	2.6	89
50	Microscopic Model of the Metalâ€“Organic Framework/Polymer Interface: A First Step toward Understanding the Compatibility in Mixed Matrix Membranes. ACS Applied Materials & Interfaces, 2016, 8, 809-819.	8.0	129
51	Hydration of a polyamide reverse-osmosis membrane. Journal of Membrane Science, 2016, 501, 248-253.	8.2	41
52	Computer modelling of the surface tension of the gasâ€“liquid and liquidâ€“liquid interface. Chemical Society Reviews, 2016, 45, 1387-1409.	38.1	167
53	Surface tension and long range corrections of cylindrical interfaces. Journal of Chemical Physics, 2015, 143, 234708.	3.0	4
54	On the structure and rejection of ions by a polyamide membrane in pressure-driven molecular dynamics simulations. Desalination, 2015, 368, 76-80.	8.2	66

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55	Theoretical Investigation of the Ionic Selectivity of Polyelectrolyte Multilayer Membranes in Nanofiltration. Langmuir, 2015, 31, 451-457.	3.5	18
56	Unravelling the anomalous dielectric permittivity of nanoconfined electrolyte solutions. Nanoscale, 2015, 7, 6661-6666.	5.6	9
57	Coarse-Graining the Liquidâ€“Liquid Interfaces with the MARTINI Force Field: How Is the Interfacial Tension Reproduced?. Journal of Chemical Theory and Computation, 2015, 11, 3818-3828.	5.3	40
58	Interfacial Structure of Toluene at an Ionic Liquid/Vapor Interface: A Molecular Dynamics Simulation Investigation. Journal of Physical Chemistry C, 2015, 119, 9966-9972.	3.1	13
59	Superpermittivity of nanoconfined water. Journal of Chemical Physics, 2015, 142, 184706.	3.0	32
60	Tunable dielectric constant of water at the nanoscale. Physical Review E, 2015, 91, 032411.	2.1	12
61	Controlling the Long-Range Corrections in Atomistic Monte Carlo Simulations of Two-Phase Systems. Journal of Chemical Theory and Computation, 2015, 11, 4573-4585.	5.3	24
62	Dielectric anisotropy of water confined into the MIL-53(Cr) metalâ€“organic framework. Molecular Simulation, 2015, 41, 483-489.	2.0	8
63	Communication: Slab thickness dependence of the surface tension: Toward a criterion of liquid sheets stability. Journal of Chemical Physics, 2014, 141, 081103.	3.0	9
64	Discotic columnar liquid crystal studied in the bulk and nanoconfined states by molecular dynamics simulation. Journal of Chemical Physics, 2014, 141, 134902.	3.0	26
65	Crossover in structure and dynamics of a primary alcohol induced by hydrogen-bonds dilution. Journal of Chemical Physics, 2014, 141, 204503.	3.0	17
66	Structure and dynamics of water confined in a polyamide reverse-osmosis membrane: A molecular-simulation study. Journal of Membrane Science, 2014, 458, 236-244.	8.2	118
67	Water confinement in nanoporous silica materials. Journal of Chemical Physics, 2014, 140, 044704.	3.0	43
68	Calculation of the surface tension of pure tin from atomistic simulations of liquidâ€“vapour systems. Molecular Physics, 2014, 112, 2654-2657.	1.7	9
69	Ultraconfinement of aqueous electrolytic solutions within hydrophilic nanotubes. RSC Advances, 2014, 4, 32755-32761.	3.6	6
70	Diffusion of Light Hydrocarbons in the Flexible MIL-53(Cr) Metalâ€“Organic Framework: A Combination of Quasi-Elastic Neutron Scattering Experiments and Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2014, 118, 14471-14477.	3.1	37
71	Thermotropic Luminescent Clustomesogen Showing a Nematic Phase: A Combination of Experimental and Molecular Simulation Studies. Chemistry - A European Journal, 2014, 20, 8561-8565.	3.3	25
72	Surface tension of spherical drops from surface of tension. Journal of Chemical Physics, 2014, 140, 034110.	3.0	16

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73	Nanoconfined gases, liquids and liquid crystals in porous materials. Molecular Simulation, 2014, 40, 698-712.	2.0	5
74	Guest-modulation of the mechanical properties of flexible porous metalâ€“organic frameworks. Journal of Materials Chemistry A, 2014, 2, 9691-9698.	10.3	18
75	Influence of the pore length on the properties of water confined in a silica nanopore. Molecular Physics, 2014, 112, 2275-2281.	1.7	6
76	Molecular simulations of polyamide reverse osmosis membranes. Desalination, 2014, 343, 48-53.	8.2	63
77	How does the electronic continuum model perform in the prediction of the surface tension of salt solutions?. Chemical Physics Letters, 2014, 595-596, 209-213.	2.6	10
78	Concentration Dependence of the Dielectric Permittivity, Structure, and Dynamics of Aqueous NaCl Solutions: Comparison between the Drude Oscillator and Electronic Continuum Models. Journal of Physical Chemistry B, 2014, 118, 3931-3940.	2.6	35
79	Quantitative Predictions of the Interfacial Tensions of Liquidâ€“Liquid Interfaces through Atomistic and Coarse Grained Models. Journal of Chemical Theory and Computation, 2014, 10, 1887-1899.	5.3	36
80	Giant optical activity of sugar in thin soap films. Journal of Colloid and Interface Science, 2013, 408, 113-116.	9.4	4
81	ZhuetÂal.Reply:. Physical Review Letters, 2013, 111, 089802.	7.8	8
82	Solvation Effects on Self-Association and Segregation Processes in tert-Butanolâ€“Aprotic Solvent Binary Mixtures. Journal of Physical Chemistry B, 2013, 117, 10221-10230.	2.6	26
83	Calculation of the surface tension of liquid copper from atomistic Monte Carlo simulations. European Physical Journal B, 2013, 86, 1.	1.5	25
84	Evaluation of MIL-47(V) for CO₂-Related Applications. Journal of Physical Chemistry C, 2013, 117, 962-970.	3.1	42
85	Recent advances in Many Body Dissipative Particles Dynamics simulations of liquid-vapor interfaces. European Physical Journal E, 2013, 36, 10.	1.6	66
86	The kinetic friction coefficient of neutral and charged polymer brushes. Soft Matter, 2013, 9, 2966.	2.7	34
87	Prediction of the concentration dependence of the surface tension and density of salt solutions: atomistic simulations using Drude oscillator polarizable and nonpolarizable models. Physical Chemistry Chemical Physics, 2013, 15, 11679.	2.8	29
88	Nanoconfined Electrolyte Solutions in Porous Hydrophilic Silica Membranes. Journal of Physical Chemistry C, 2013, 117, 11017-11027.	3.1	40
89	Confinement of tert-Butanol Nanoclusters in Hydrophilic and Hydrophobic Silica Nanopores. Journal of Physical Chemistry C, 2013, 117, 15203-15212.	3.1	49
90	Molecular modeling of the liquid-vapor interfaces of a multi-component mixture: Prediction of the coexisting densities and surface tensions at different pressures and gas compositions. Journal of Chemical Physics, 2013, 139, 024701.	3.0	22

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91	Microscopic insight into the nanocoalescence of a water droplet on a water bath. Europhysics Letters, 2013, 104, 46004.	2.0	1
92	Local description of surface tension through thermodynamic and mechanical definitions. Molecular Simulation, 2013, 39, 603-611.	2.0	14
93	Anomalous Dielectric Behavior of Nanoconfined Electrolytic Solutions. Physical Review Letters, 2012, 109, 107801.	7.8	64
94	Computation of the hindrance factor for the diffusion for nanoconfined ions: molecular dynamics simulations versus continuum-based models. Molecular Physics, 2012, 110, 1107-1114.	1.7	12
95	Calculation of local dielectric permittivity of confined liquids from spatial dipolar correlations. Europhysics Letters, 2012, 99, 37008.	2.0	33
96	Ion Transport in Nanoporous Membranes. Procedia Engineering, 2012, 44, 2048-2050.	1.2	0
97	REMOVED: Hindered Diffusion of Ions Confined in Nanopores: Molecular Dynamics Simulations Versus Continuumâ€“Based Models. Procedia Engineering, 2012, 44, 2088-2089.	1.2	0
98	Guest dependent pressure behavior of the flexible MIL-53(Cr): A computational exploration. Dalton Transactions, 2012, 41, 3915-3919.	3.3	38
99	Comparative Guest, Thermal, and Mechanical Breathing of the Porous Metal Organic Framework MIL-53(Cr): A Computational Exploration Supported by Experiments. Journal of Physical Chemistry C, 2012, 116, 13289-13295.	3.1	90
100	Theoretical Hydrogen Cryostorage in Doped MIL-101(Cr) Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2012, 116, 10504-10509.	3.1	30
101	Separation of CO2â€“CH4 mixtures in the mesoporous MIL-100(Cr) MOF: experimental and modelling approaches. Dalton Transactions, 2012, 41, 4052.	3.3	78
102	Frictional forces in polyelectrolyte brushes: effects of sliding velocity, solvent quality and salt. Soft Matter, 2012, 8, 4635.	2.7	36
103	Calculation of the surface tension and pressure components from a non-exponential perturbation method of the thermodynamic route. Journal of Chemical Physics, 2012, 136, 024104.	3.0	32
104	Large breathing of the MOF MIL-47(VIV) under mechanical pressure: a joint experimentalâ€“modelling exploration. Chemical Science, 2012, 3, 1100.	7.4	176
105	Coarse Grained Simulations of the Electrolytes at the Waterâ€“Air Interface from Many Body Dissipative Particle Dynamics. Journal of Chemical Theory and Computation, 2012, 8, 787-791.	5.3	50
106	Hydrogen-Bond-Induced Supermolecular Assemblies in a Nanoconfined Tertiary Alcohol. Journal of Physical Chemistry C, 2011, 115, 17761-17767.	3.1	28
107	Exploration of the Long-Chain N-Alkanes Adsorption and Diffusion in the MOF-Type MIL-47 (V) Material by Combining Experimental and Molecular Simulation Tools. Journal of Physical Chemistry C, 2011, 115, 13868-13876.	3.1	49
108	Local pressure components and surface tension of spherical interfaces. Thermodynamic versus mechanical definitions. I. A mesoscale modeling of droplets. Journal of Chemical Physics, 2011, 135, 104105.	3.0	23

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109	Configurational temperature and local properties of the anisotropic Gayâ€“Berne liquid crystal model: Applications to the isotropic liquid/vapor interface and isotropic/nematic transition. Journal of Chemical Physics, 2011, 134, 034116.	3.0	7
110	Adsorption of n-alkane vapours at the water surface. Physical Chemistry Chemical Physics, 2011, 13, 11308.	2.8	18
111	Surface tension of waterâ€“alcohol mixtures from Monte Carlo simulations. Journal of Chemical Physics, 2011, 134, 044709.	3.0	81
112	Molecular Insight into the Adsorption of H₂S in the Flexible MIL-53(Cr) and Rigid MIL-47(V) MOFs: Infrared Spectroscopy Combined to Molecular Simulations. Journal of Physical Chemistry C, 2011, 115, 2047-2056.	3.1	157
113	Prediction of the Surface Tension of the Liquidâ^'Vapor Interface of Alcohols from Monte Carlo Simulations. Journal of Physical Chemistry C, 2011, 115, 8670-8683.	3.1	42
114	Molecular simulations of confined liquids: An alternative to the grand canonical Monte Carlo simulations. Journal of Chemical Physics, 2011, 134, 074104.	3.0	40
115	Mesoscale modeling of the water liquid-vapor interface: A surface tension calculation. Physical Review E, 2011, 83, 051601.	2.1	83
116	The non-Gaussian dynamics of glycerol. Journal of Physics Condensed Matter, 2011, 23, 505102.	1.8	10
117	Unusual Chainâ€Length Dependence of the Diffusion of nâ€Alkanes in the Metalâ€“Organic Framework MILâ€47(V): The Blowgun Effect. Chemistry - A European Journal, 2010, 16, 10337-10341.	3.3	42
118	Toward a Coarse Graining/All Atoms Force Field (CG/AA) from a Multiscale Optimization Method: An Application to the MCM-41 Mesoporous Silicates. Journal of Chemical Theory and Computation, 2010, 6, 3212-3222.	5.3	20
119	Hybrid Monte Carlo Simulations Combined with a Phase Mixture Model to Predict the Structural Transitions of a Porous Metalâ^'Organic Framework Material upon Adsorption of Guest Molecules. Journal of Physical Chemistry C, 2010, 114, 6496-6502.	3.1	112
120	Physics Behind the Guest-Assisted Structural Transitions of a Porous Metalâ^'Organic Framework Material. Journal of Physical Chemistry Letters, 2010, 1, 2810-2815.	4.6	59
121	Calculation of the surface tension from multibody dissipative particle dynamics and Monte Carlo methods. Physical Review E, 2010, 82, 016706.	2.1	52
122	Adsorption of light hydrocarbons in the flexible MIL-53(Cr) and rigid MIL-47(V) metalâ€“organic frameworks: a combination of molecular simulations and microcalorimetry/gravimetry measurements. Physical Chemistry Chemical Physics, 2010, 12, 6428.	2.8	82
123	Numerical evidence of the formation of a thin microscopic film of methane at the water surface: a free energy calculation. Physical Chemistry Chemical Physics, 2010, 12, 5203.	2.8	32
124	Transport Diffusivity of CO₂ in the Highly Flexible Metalâ€“Organic Framework MILâ€53(Cr). Angewandte Chemie - International Edition, 2009, 48, 8335-8339.	13.8	109
125	Adsorption of CO2, CH4 and their binary mixture in Faujasite NaY: A combination of molecular simulations with gravimetryâ€“manometry and microcalorimetry measurements. Microporous and Mesoporous Materials, 2009, 119, 117-128.	4.4	86
126	Pore dimensionality effects on the dynamics of a nanoconfined liquid-crystal. Chemical Physics Letters, 2009, 482, 234-238.	2.6	14

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127	Calculation of the surface tension of cyclic and aromatic hydrocarbons from Monte Carlo simulations using an anisotropic united atom model (AUA). Physical Chemistry Chemical Physics, 2009, 11, 6132.	2.8	32
128	Co-adsorption and Separation of CO₂â"CH₄ Mixtures in the Highly Flexible MIL-53(Cr) MOF. Journal of the American Chemical Society, 2009, 131, 17490-17499.	13.7	398
129	Monte Carlo Simulations of the Pressure Dependence of the Waterâ"Acid Gas Interfacial Tensions. Journal of Physical Chemistry B, 2009, 113, 14277-14290.	2.6	58
130	Monte Carlo calculation of the methane-water interfacial tension at high pressures. Journal of Chemical Physics, 2009, 131, 124707.	3.0	65
131	Calculation of the surface tension from Monte Carlo simulations: Does the model impact on the finite-size effects?. Journal of Chemical Physics, 2009, 130, 184710.	3.0	82
132	Quasiâ€Elastic Neutron Scattering and Molecular Dynamics Study of Methane Diffusion in Metal Organic Frameworks MILâ€47(V) and MILâ€53(Cr). Angewandte Chemie - International Edition, 2008, 47, 6611-6615.	13.8	154
133	Molecular Dynamics Simulations of Breathing MOFs: Structural Transformations of MILâ€53(Cr) upon Thermal Activation and CO₂ Adsorption. Angewandte Chemie - International Edition, 2008, 47, 8487-8491.	13.8	302
134	Surface Tensions of Linear and Branched Alkanes from Monte Carlo Simulations Using the Anisotropic United Atom Model. Journal of Physical Chemistry B, 2008, 112, 13885-13897.	2.6	49
135	Optimisation of the dynamical behaviour of the anisotropic united atom model of branched alkanes: application to the molecular simulation of fuel gasoline. Molecular Simulation, 2008, 34, 211-230.	2.0	24
136	Expressions for local contributions to the surface tension from the virial route. Physical Review E, 2008, 77, 031601.	2.1	64
137	Surface tension of water and acid gases from Monte Carlo simulations. Journal of Chemical Physics, 2008, 128, 154716.	3.0	84
138	Multiple histogram reweighting method for the surface tension calculation. Journal of Chemical Physics, 2008, 128, 154718.	3.0	42
139	Molecular simulations of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-alkane liquid-vapor interface: Interfacial properties and their long range corrections. Physical Review E, 2007, 75, 051602.	2.1	97
140	Computational and Experimental Investigations of Supramolecular Assemblies of p-Sulfonatocalix[4]arene Organized by Weak Forces. Journal of Physical Chemistry B, 2007, 111, 11478-11485.	2.6	9
141	Methodology for the Calculation of the Potential of Mean Force for a Cationâ€"Ï€ Complex in Water. ChemPhysChem, 2007, 8, 1648-1656.	2.1	8
142	Entropy and enthalpy calculations from perturbation and integration thermodynamics methods using molecular dynamics simulations: applications to the calculation of hydration and association thermodynamic properties. Molecular Physics, 2006, 104, 2929-2943.	1.7	47
143	Calculation of the absolute thermodynamic properties of association of host-guest systems from the intermolecular potential of mean force. Journal of Chemical Physics, 2006, 125, 224503.	3.0	11
144	Calculations of the potential of mean force from molecular dynamics simulations using different methodologies: an application to the determination of the binding thermodynamic properties of an ion pair. Molecular Physics, 2006, 104, 3787-3799.	1.7	14

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145	MD Simulations of the Binding of Alcohols and Diols by a Calixarene in Water:â€‰ Connections between Microscopic and Macroscopic Properties. Journal of Physical Chemistry B, 2005, 109, 23579-23587.	2.6	25
146	Structures and Energetics of Complexes of the p-Sulfonatocalix[4]arene with Ammonium, Alkylammonium, and Tetraalkylammonium Cations in Water Using Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2004, 108, 5095-5104.	2.6	41
147	Gibbs Free Energy Perturbation Calculations:â€‰ An Application to the Binding of Alkylammonium Cations by a Water-Soluble Calixarene. Journal of Physical Chemistry B, 2004, 108, 11744-11752.	2.6	35
148	Water transport through a two-dimensional nanoporous material: is there a relationship between water flux and surface tension?. Molecular Physics, 0, , .	1.7	0