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	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
2	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
3	Large breathing of the MOF MIL-47(VIV) under mechanical pressure: a joint experimentalâ€"modelling exploration. Chemical Science, 2012, 3, 1100.	7.4	176
4	Computer modelling of the surface tension of the gasâ€"liquid and liquidâ€"liquid interface. Chemical Society Reviews, 2016, 45, 1387-1409.	38.1	167
5	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
6	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
7	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
8	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
9	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
10	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
11	Electrically Induced Breathing of the MIL-53(Cr) Metalâ€"Organic Framework. ACS Central Science, 2017, 3, 394-398.	11.3	102
12	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
13	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
14	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
15	Tailoring the separation properties of flexible metal-organic frameworks using mechanical pressure. Nature Communications, 2020, 11, 1216.	12.8	88
16	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
17	Surface tension of water and acid gases from Monte Carlo simulations. Journal of Chemical Physics, 2008, 128, 154716.	3.0	84
18	Mesoscale modeling of the water liquid-vapor interface: A surface tension calculation. Physical Review E, 2011, 83, 051601.	2.1	83

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19	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
20	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
21	Surface tension of waterâ€“alcohol mixtures from Monte Carlo simulations. Journal of Chemical Physics, 2011, 134, 044709.	3.0	81
22	Separation of CO2â€“CH4 mixtures in the mesoporous MIL-100(Cr) MOF: experimental and modelling approaches. Dalton Transactions, 2012, 41, 4052.	3.3	78
23	Physics behind Water Transport through Nanoporous Boron Nitride and Graphene. Journal of Physical Chemistry Letters, 2016, 7, 3371-3376.	4.6	70
24	Recent advances in Many Body Dissipative Particles Dynamics simulations of liquid-vapor interfaces. European Physical Journal E, 2013, 36, 10.	1.6	66
25	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
26	Monte Carlo calculation of the methane-water interfacial tension at high pressures. Journal of Chemical Physics, 2009, 131, 124707.	3.0	65
27	Expressions for local contributions to the surface tension from the virial route. Physical Review E, 2008, 77, 031601.	2.1	64
28	Anomalous Dielectric Behavior of Nanoconfined Electrolytic Solutions. Physical Review Letters, 2012, 109, 107801.	7.8	64
29	Molecular simulations of polyamide reverse osmosis membranes. Desalination, 2014, 343, 48-53.	8.2	63
30	Ultrafast diffusion of Ionic Liquids Confined in Carbon Nanotubes. Scientific Reports, 2016, 6, 28518.	3.3	62
31	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
32	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
33	Calculation of the surface tension from multibody dissipative particle dynamics and Monte Carlo methods. Physical Review E, 2010, 82, 016706.	2.1	52
34	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
35	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
36	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

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37	Confinement of tert-Butanol Nanoclusters in Hydrophilic and Hydrophobic Silica Nanopores. Journal of Physical Chemistry C, 2013, 117, 15203-15212.	3.1	49
38	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
39	Water confinement in nanoporous silica materials. Journal of Chemical Physics, 2014, 140, 044704.	3.0	43
40	Multiple histogram reweighting method for the surface tension calculation. Journal of Chemical Physics, 2008, 128, 154718.	3.0	42
41	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
42	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
43	Evaluation of MIL-47(V) for CO₂-Related Applications. Journal of Physical Chemistry C, 2013, 117, 962-970.	3.1	42
44	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
45	Hydration of a polyamide reverse-osmosis membrane. Journal of Membrane Science, 2016, 501, 248-253.	8.2	41
46	Molecular simulations of confined liquids: An alternative to the grand canonical Monte Carlo simulations. Journal of Chemical Physics, 2011, 134, 074104.	3.0	40
47	Nanoconfined Electrolyte Solutions in Porous Hydrophilic Silica Membranes. Journal of Physical Chemistry C, 2013, 117, 11017-11027.	3.1	40
48	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
49	Guest dependent pressure behavior of the flexible MIL-53(Cr): A computational exploration. Dalton Transactions, 2012, 41, 3915-3919.	3.3	38
50	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
51	Frictional forces in polyelectrolyte brushes: effects of sliding velocity, solvent quality and salt. Soft Matter, 2012, 8, 4635.	2.7	36
52	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
53	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
54	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

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55	The kinetic friction coefficient of neutral and charged polymer brushes. Soft Matter, 2013, 9, 2966.	2.7	34
56	Calculation of local dielectric permittivity of confined liquids from spatial dipolar correlations. Europhysics Letters, 2012, 99, 37008.	2.0	33
57	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
58	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
59	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
60	Superpermittivity of nanoconfined water. Journal of Chemical Physics, 2015, 142, 184706.	3.0	32
61	Nanofiltration performance of conical and hourglass nanopores. Journal of Membrane Science, 2018, 552, 336-340.	8.2	32
62	Theoretical Hydrogen Cryostorage in Doped MIL-101(Cr) Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2012, 116, 10504-10509.	3.1	30
63	Pressure-driven molecular dynamics simulations of water transport through a hydrophilic nanochannel. Molecular Physics, 2016, 114, 2655-2663.	1.7	30
64	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
65	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
66	Hydrogen-Bond-Induced Supermolecular Assemblies in a Nanoconfined Tertiary Alcohol. Journal of Physical Chemistry C, 2011, 115, 17761-17767.	3.1	28
67	High Water Flux with Ions Sieving in a Desalination 2D Sub-Nanoporous Boron Nitride Material. ACS Omega, 2018, 3, 6305-6310.	3.5	28
68	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
69	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
70	Calculation of the interfacial tension of the graphene-water interaction by molecular simulations. Journal of Chemical Physics, 2019, 150, 014703.	3.0	26
71	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
72	Calculation of the surface tension of liquid copper from atomistic Monte Carlo simulations. European Physical Journal B, 2013, 86, 1.	1.5	25

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73	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
74	Dynamics of water confined in mesopores with variable surface interaction. Journal of Chemical Physics, 2021, 154, 094505.	3.0	25
75	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
76	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
77	Microphase Separation of Binary Liquids Confined in Cylindrical Pores. Journal of Physical Chemistry C, 2016, 120, 9245-9252.	3.1	24
78	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
79	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
80	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
81	Water nano-diffusion through the Nafion fuel cell membrane. Journal of Membrane Science, 2020, 602, 117958.	8.2	21
82	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
83	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
84	Microstructure of nonideal methanol binary liquid mixtures. Physical Review E, 2019, 99, 062607.	2.1	20
85	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
86	Calculation of the surface tension of water: 40 years of molecular simulations. Molecular Simulation, 2019, 45, 295-303.	2.0	19
87	Adsorption of n-alkane vapours at the water surface. Physical Chemistry Chemical Physics, 2011, 13, 11308.	2.8	18
88	Guest-modulation of the mechanical properties of flexible porous metalâ€“organic frameworks. Journal of Materials Chemistry A, 2014, 2, 9691-9698.	10.3	18
89	Theoretical Investigation of the Ionic Selectivity of Polyelectrolyte Multilayer Membranes in Nanofiltration. Langmuir, 2015, 31, 451-457.	3.5	18
90	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

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91	Crossover in structure and dynamics of a primary alcohol induced by hydrogen-bonds dilution. Journal of Chemical Physics, 2014, 141, 204503.	3.0	17
92	The extent of the glass transition from molecular simulation revealing an overcrank effect. Journal of Computational Chemistry, 2018, 39, 255-261.	3.3	17
93	Surface tension of spherical drops from surface of tension. Journal of Chemical Physics, 2014, 140, 034110.	3.0	16
94	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
95	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
96	Pore dimensionality effects on the dynamics of a nanoconfined liquid-crystal. Chemical Physics Letters, 2009, 482, 234-238.	2.6	14
97	Local description of surface tension through thermodynamic and mechanical definitions. Molecular Simulation, 2013, 39, 603-611.	2.0	14
98	Test-area surface tension calculation of the graphene-methane interface: Fluctuations and commensurability. Journal of Chemical Physics, 2017, 146, 214112.	3.0	14
99	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
100	Molecular Origin of the Prepeak in the Structure Factor of Alcohols. Journal of Physical Chemistry B, 2020, 124, 11501-11509.	2.6	14
101	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
102	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
103	Tunable dielectric constant of water at the nanoscale. Physical Review E, 2015, 91, 032411.	2.1	12
104	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
105	Microphase separation of a miscible binary liquid mixture under confinement at the nanoscale. Npj Computational Materials, 2019, 5, .	8.7	12
106	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
107	Importance of the tail corrections on surface tension of curved liquid-vapor interfaces. Journal of Chemical Physics, 2017, 146, 084703.	3.0	11
108	The non-Gaussian dynamics of glycerol. Journal of Physics Condensed Matter, 2011, 23, 505102.	1.8	10

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109	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
110	Symmetry breakings in a metal organic framework with a confined guest. Physical Review B, 2020, 101, .	3.2	10
111	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
112	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
113	Calculation of the surface tension of pure tin from atomistic simulations of liquidâ€“vapour systems. Molecular Physics, 2014, 112, 2654-2657.	1.7	9
114	Unravelling the anomalous dielectric permittivity of nanoconfined electrolyte solutions. Nanoscale, 2015, 7, 6661-6666.	5.6	9
115	Tuning the hexane isomer separation performances of Zeolitic Imidazole Framework-8 using mechanical pressure. Journal of Chemical Physics, 2021, 154, 084702.	3.0	9
116	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
117	ZhuetÂal.Reply:. Physical Review Letters, 2013, 111, 089802.	7.8	8
118	Dielectric anisotropy of water confined into the MIL-53(Cr) metalâ€“organic framework. Molecular Simulation, 2015, 41, 483-489.	2.0	8
119	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
120	Dynamic Heterogeneities in Liquid Mixtures Confined in Nanopores. Journal of Physical Chemistry B, 2020, 124, 3152-3162.	2.6	8
121	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
122	Is Fineâ€Grained Simulation Able to Propose New Polyelectrolyte Membranes?. Fuel Cells, 2016, 16, 675-681.	2.4	7
123	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
124	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
125	Ultraconfinement of aqueous electrolytic solutions within hydrophilic nanotubes. RSC Advances, 2014, 4, 32755-32761.	3.6	6
126	Influence of the pore length on the properties of water confined in a silica nanopore. Molecular Physics, 2014, 112, 2275-2281.	1.7	6

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127	Associated molecular liquids at the graphene monolayer interface. Journal of Chemical Physics, 2021, 154, 104504.	3.0	6
128	Nanoconfined gases, liquids and liquid crystals in porous materials. Molecular Simulation, 2014, 40, 698-712.	2.0	5
129	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
130	Anomalous Dynamics of a Nanoconfined Gas in a Soft Metalâ€“Organics Framework. Journal of Physical Chemistry Letters, 2019, 10, 1698-1708.	4.6	5
131	Computational Assessment of Water Desalination Performance of Multiâ€Walled Carbon Nanotubes. Advanced Theory and Simulations, 2020, 3, 1900254.	2.8	5
132	Giant optical activity of sugar in thin soap films. Journal of Colloid and Interface Science, 2013, 408, 113-116.	9.4	4
133	Surface tension and long range corrections of cylindrical interfaces. Journal of Chemical Physics, 2015, 143, 234708.	3.0	4
134	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
135	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
136	Radial-based tail methods for Monte Carlo simulations of cylindrical interfaces. Journal of Chemical Physics, 2018, 148, 094702.	3.0	2
137	Interfacial tension of the grapheneâ€“water solidâ€“liquid interface: how to handle the electrostatic interactions?. Molecular Physics, 2021, 119, .	1.7	2
138	Interactions between methanol/toluene binary mixtures and an organic solvent nanofiltration PIM-1 membrane. Journal of Molecular Liquids, 2022, 357, 119146.	4.9	2
139	Microscopic insight into the nanocoalescence of a water droplet on a water bath. Europhysics Letters, 2013, 104, 46004.	2.0	1
140	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
141	Numerical evidence of heterogeneity and nanophases in a binary liquid confined at the nanoscale. Molecular Simulation, 2018, 44, 728-735.	2.0	1
142	Ion Transport in Nanoporous Membranes. Procedia Engineering, 2012, 44, 2048-2050.	1.2	0
143	REMOVED: Hindered Diffusion of Ions Confined in Nanopores: Molecular Dynamics Simulations Versus Continuumâ€“Based Models. Procedia Engineering, 2012, 44, 2088-2089.	1.2	0
144	Anomalous dynamics of water at the octopeptide lanreotide surface. RSC Advances, 2020, 10, 33903-33910.	3.6	0

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145	Static dielectric permittivity of ionic liquids ultraconfined in carbon nanotubes. Nano Express, 2021, 2, 010036.	2.4	0
146	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
147	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
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