Carlos Nieto-Draghi

List of Publications by Year
in descending order

61 papers	2,538 citations	230014 27 h-index	214428 50 g-index
62 all docs	62 docs citations	62 times ranked	3419 citing authors

#	Article	IF	Citations
1	Impact of Electrolytes on Produced Water Destabilization. Energy & Fuels, 2022, 36, 1271-1282.	2.5	1
2	Impact of adsorption kinetics on pollutant dispersion in water flowing in nanopores: A Lattice Boltzmann approach to stationary and transient conditions. Advances in Water Resources, 2022, 162, 104143.	1.7	2
3	Impact of Organic Templates on the Selective Formation of Zeolite Oligomers. Angewandte Chemie - International Edition, 2021, 60, 7111-7116.	7.2	7
4	Impact of Organic Templates on the Selective Formation of Zeolite Oligomers. Angewandte Chemie, 2021, 133, 7187-7192.	1.6	9
5	RÃ¼cktitelbild: Impact of Organic Templates on the Selective Formation of Zeolite Oligomers (Angew.) Tj ETQq1 1 0.784314 rgBT /Ov	1.6	0
6	Experimental and Mesoscopic Modeling Study of Water/Crude Oil Interfacial Tension. Energy & Fuels, 2021, 35, 11858-11868.	2.5	5
7	Lattice Boltzmann method for adsorption under stationary and transient conditions: Interplay between transport and adsorption kinetics in porous media. Physical Review E, 2021, 104, 015314.	0.8	5
8	Comparisons of Molecular Structure Generation Methods Based on Fragment Assemblies and Genetic Graphs. Journal of Chemical Information and Modeling, 2021, 61, 4245-4258.	2.5	7
9	Inverseâ€QSPR for de novo Design: A Review. Molecular Informatics, 2020, 39, e1900087.	1.4	27
10	Cooperative Effects Dominating the Thermodynamics and Kinetics of Surfactant Adsorption in Porous Media: From Lateral Interactions to Surface Aggregation. Journal of Physical Chemistry B, 2020, 124, 10841-10849.	1.2	3
11	A Multi-Scale Modeling of Confined Fluid: from Nanopore to Unconventional Reservoir Simulation. Journal of Petroleum Science and Engineering, 2020, 193, 107364.	2.1	4
12	Phase behavior of hydrocarbons in nano-pores. Fluid Phase Equilibria, 2019, 497, 104-121.	1.4	25
13	Thermodynamically Consistent Force Field for Coarse-Grained Modeling of Aqueous Electrolyte Solution. Journal of Physical Chemistry B, 2019, 123, 2424-2431.	1.2	6
14	Thermodynamic study of binary systems containing sulphur dioxide and nitric oxide: Measurements and modelling. Fluid Phase Equilibria, 2018, 461, 84-100.	1.4	7
15	Simulations of Interfacial Tension of Liquidâ€“Liquid Ternary Mixtures Using Optimized Parametrization for Coarse-Grained Models. Journal of Chemical Theory and Computation, 2018, 14, 4438-4454.	2.3	6
16	Mineral- and Ion-Specific Effects at Clayâ€“Water Interfaces: Structure, Diffusion, and Hydrodynamics. Journal of Physical Chemistry C, 2018, 122, 18484-18492.	1.5	34
17	Diffusion under Confinement: Hydrodynamic Finite-Size Effects in Simulation. Journal of Chemical Theory and Computation, 2017, 13, 2881-2889.	2.3	81
18	New Molecular Simulation Method To Determine Both Aluminum and Cation Location in Cationic Zeolites. Chemistry of Materials, 2017, 29, 513-523.	3.2	34

#	Article	IF	Citations
19	Aspects of Asphaltene Aggregation Obtained from Coarse-Grained Molecular Modeling. Energy & Fuels, 2015, 29, 556-566.	2.5	24
20	Surface Photografting of Acrylic Acid on Poly(dimethylsiloxane). Experimental and Dissipative Particle Dynamics Studies. Langmuir, 2015, 31, 1400-1409.	1.6	13
21	A General Guidebook for the Theoretical Prediction of Physicochemical Properties of Chemicals for Regulatory Purposes. Chemical Reviews, 2015, 115, 13093-13164.	23.0	116
22	A Kinetic Monte Carlo Simulation Study of Synthesis Variables and Diffusion Coefficients in Early Stages of Silicate Oligomerization. Journal of Physical Chemistry C, 2015, 119, 28871-28884.	1.5	18
23	Modeling of Zeolitic-Like Hybrid Materials for Gas Separation. , 2015, , 381-418.		0
24	Equilibrium and Transport Properties of Primary, Secondary and Tertiary Amines by Molecular Simulation. Oil and Gas Science and Technology, 2014, 69, 833-849.	1.4	7
25	Molecular simulation of zeolite flexibility. Molecular Simulation, 2014, 40, 6-15.	0.9	21
26	Impact of functionalized linkers on the energy landscape of ZIFs. CrystEngComm, 2013, 15, 9603.	1.3	28
27	A Transferable Force Field for Primary, Secondary, and Tertiary Alkanolamines. Journal of Chemical Theory and Computation, 2013, 9, 2097-2103.	2.3	26
28	Transferable Force Field for Equilibrium and Transport Properties in Linear and Branched Monofunctional and Multifunctional Amines. II. Secondary and Tertiary Amines. Journal of Physical Chemistry B, 2012, 116, 6193-6202.	1.2	18
29	Molecular Modeling of Diffusion Coefficient and Ionic Conductivity of CO₂ in Aqueous Ionic Solutions. Journal of Physical Chemistry B, 2012, 116, 2787-2800.	1.2	23
30	Composition Analysis and Viscosity Prediction of Complex Fuel Mixtures Using a Molecular-Based Approach. Energy & Fuels, 2012, 26, 2220-2230.	2.5	38
31	Prediction of thermodynamic properties of adsorbed gases in zeolitic imidazolate frameworks. RSC Advances, 2012, 2, 6028.	1.7	46
32	Prediction of Surfactantsâ€™ Properties using Multiscale Molecular Modeling Tools: A Review. Oil and Gas Science and Technology, 2012, 67, 969-982.	1.4	47
33	Experimental and Computational Study of Functionality Impact on Sodaliteâ€“Zeolitic Imidazolate Frameworks for CO₂Separation. Journal of Physical Chemistry C, 2011, 115, 16425-16432.	1.5	128
34	Transferable Force Field for Equilibrium and Transport Properties in Linear, Branched, and Bifunctional Amines I. Primary Amines. Journal of Physical Chemistry B, 2011, 115, 14617-14625.	1.2	23
35	Guest-induced gate-opening of a zeolite imidazolate framework. New Journal of Chemistry, 2011, 35, 546-550.	1.4	172
36	Facile synthesis of an ultramicroporous MOF tubular membrane with selectivity towards CO₂. New Journal of Chemistry, 2011, 35, 41-44.	1.4	125

#	Article	IF	Citations
37	Adsorption of CO₂, CH₄, and N₂ on Zeolitic Imidazolate Frameworks: Experiments and Simulations. Chemistry - A European Journal, 2010, 16, 1560-1571.	1.7	344
38	Extension of a Charged Anisotropic United Atoms Model to Polycyclic Aromatic Compounds. Journal of Physical Chemistry B, 2010, 114, 6522-6530.	1.2	15
39	A molecular simulation study of the distribution of cation inÂzeolites. Adsorption, 2008, 14, 743-754.	1.4	32
40	Diffusion Coefficients in CO₂/n-Alkane Binary Liquid Mixtures by Molecular Simulation. Journal of Physical Chemistry B, 2008, 112, 16610-16618.	1.2	47
41	Prediction of Transport Properties by Molecular Simulation: Methanol and Ethanol and Their Mixture. Journal of Physical Chemistry B, 2008, 112, 16664-16674.	1.2	106
42	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.	0.9	24
43	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
44	Molecular Dynamics Simulation of Acid Gas Mixtures:â€‰ A Comparison between Several Approximations. Industrial & Engineering Chemistry Research, 2007, 46, 5238-5244.	1.8	36
45	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
46	Thermodynamic and transport properties of carbon dioxide from molecular simulation. Journal of Chemical Physics, 2007, 126, 064509.	1.2	76
47	Anisotropic United Atom Model Including the Electrostatic Interactions of Benzene. Journal of Physical Chemistry B, 2007, 111, 3730-3741.	1.2	38
48	Molecular simulation applied to fluid properties in the oil and gas industry. Molecular Simulation, 2007, 33, 287-304.	0.9	34
49	Molecular simulation of the thermophysical properties of fluids: From understanding toward quantitative predictions. Journal of Molecular Liquids, 2007, 134, 71-89.	2.3	99
50	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
51	Polyoxometalates in Solution: Molecular Dynamics Simulations on the ?-PW12O403- Keggin Anion in Aqueous Media.. ChemInform, 2005, 36, no.	0.1	0
52	Histogram Reweighting Method for Dynamic Properties. Physical Review Letters, 2005, 95, 040603.	2.9	8
53	Structure and dynamics of water in aqueous methanol. Journal of Physics Condensed Matter, 2005, 17, S3265-S3272.	0.7	13
54	Computing the Soret coefficient in aqueous mixtures using boundary driven nonequilibrium molecular dynamics. Journal of Chemical Physics, 2005, 122, 114503.	1.2	50

#	Article	IF	Citations
55	Polyoxometalates in Solution:â€‰ Molecular Dynamics Simulations on the Î±-PW12O403- Keggin Anion in Aqueous Media. Journal of Physical Chemistry A, 2005, 109, 1216-1222.	1.1	96
56	Transport coefficients and dynamic properties of hydrogen sulfide from molecular simulation. Journal of Chemical Physics, 2005, 123, 014505.	1.2	21
57	The role of molecular interactions in the change of sign of the Soret coefficient. Europhysics Letters, 2004, 67, 976-982.	0.7	40
58	Dynamical and structural properties of benzene in supercritical water. Journal of Chemical Physics, 2004, 121, 10566-10576.	1.2	27
59	Dynamic and structural behavior of different rigid nonpolarizable models of water. Journal of Chemical Physics, 2003, 118, 7954-7964.	1.2	49
60	Non-equilibrium momentum exchange algorithm for molecular dynamics simulation of heat flow in multicomponent systems. Molecular Physics, 2003, 101, 2303-2307.	0.8	74
61	Transport properties of dimethyl sulfoxide aqueous solutions. Journal of Chemical Physics, 2003, 119, 4782-4789.	1.2	59