Jose Manuel Miguez Diaz

List of Publications by Year
in descending order

25 papers	562 citations	759233 12 h-index	610901 24 g-index
25 all docs	25 docs citations	25 times ranked	442 citing authors

#	Article	IF	Citations
1	Molecular dynamics of liquidâ€“liquid equilibrium and interfacial properties of aqueous solutions of methyl esters. Physical Chemistry Chemical Physics, 2022, 24, 5371-5382.	2.8	1
2	Phase equilibria and interfacial properties of selected methaneÂ+Ân-alkane binary mixtures. Journal of Molecular Liquids, 2021, 341, 116918.	4.9	6
3	Molecular modelling techniques for predicting liquidâ€“liquid interfacial properties of methanol plus alkane (n-hexane, n-heptane, n-octane) mixtures. Physical Chemistry Chemical Physics, 2020, 22, 27121-27133.	2.8	3
4	Preferential Orientations and Anomalous Interfacial Tensions in Aqueous Solutions of Alcohols. Journal of Physical Chemistry B, 2020, 124, 8388-8401.	2.6	3
5	Vapourâ€“liquid phase equilibria and interfacial properties of fatty acid methyl esters from molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 4974-4983.	2.8	11
6	Phase Equilibria and Interfacial Properties of the Tetrahydrofuran + Methane Binary Mixture from Experiment and Computer Simulation. Journal of Physical Chemistry C, 2019, 123, 20960-20970.	3.1	12
7	On the Physical Insight into the Barotropic Effect in the Interfacial Behavior for the H₂O + CO₂ Mixture. Journal of Physical Chemistry C, 2019, 123, 28123-28130.	3.1	21
8	An accurate density functional theory for the vaporâ€“liquid interface of chain molecules based on the statistical associating fluid theory for potentials of variable range for Mie chainlike fluids. Physical Chemistry Chemical Physics, 2019, 21, 11937-11948.	2.8	4
9	Interfacial Properties of Tetrahydrofuran and Carbon Dioxide Mixture from Computer Simulation. Journal of Physical Chemistry C, 2018, 122, 16142-16153.	3.1	7
10	Adsorption and interfacial phenomena of a Lennard-Jones fluid adsorbed in slit pores: DFT and GCMC simulations. Molecular Physics, 2018, 116, 3417-3424.	1.7	1
11	Measurement and modeling of high pressure density and interfacial tension of carbon dioxide + tetrahydrofuran mixture. Journal of Supercritical Fluids, 2017, 128, 359-369.	3.2	4
12	Vapourâ€“liquid interfacial properties of square-well chains from density functional theory and Monte Carlo simulation. Physical Chemistry Chemical Physics, 2017, 19, 12296-12309.	2.8	12
13	Computational study of the interplay between intermolecular interactions and CO₂orientations in type I hydrates. Physical Chemistry Chemical Physics, 2017, 19, 3384-3393.	2.8	17
14	On interfacial properties of tetrahydrofuran: Atomistic and coarse-grained models from molecular dynamics simulation. Journal of Chemical Physics, 2016, 144, 144702.	3.0	13
15	Molecular dynamics simulation of CO2 hydrates: Prediction of three phase coexistence line. Journal of Chemical Physics, 2015, 142, 124505.	3.0	96
16	Understanding the Phase Behavior of Tetrahydrofuran + Carbon Dioxide, + Methane, and + Water Binary Mixtures from the SAFT-VR Approach. Journal of Physical Chemistry B, 2015, 119, 14288-14302.	2.6	17
17	Nonlocal Density Functional Theory and Grand Canonical Monte Carlo Molecular Simulations of Water Adsorption in Confined Media. Journal of Physical Chemistry C, 2014, 118, 24905-24914.	3.1	20
18	Comprehensive Characterization of Interfacial Behavior for the Mixture CO₂ + H₂O + CH₄: Comparison between Atomistic and Coarse Grained Molecular Simulation Models and Density Gradient Theory. Journal of Physical Chemistry C, 2014, 118, 24504-24519.	3.1	52

#	Article	IF	Citations
19	Influence of the long-range corrections on the interfacial properties of molecular models using Monte Carlo simulation. Journal of Chemical Physics, 2013, 138, 034707.	3.0	52
20	On interfacial tension calculation from the test-area methodology in the grand canonical ensemble. Journal of Chemical Physics, 2012, 136, 114707.	3.0	9
21	Vapor-liquid interfacial properties of rigid-linear Lennard-Jones chains. Journal of Chemical Physics, 2012, 137, 084706.	3.0	21
22	Solidâ^'Solid and Solidâ^'Fluid Equilibria of the Most Popular Models of Methanol Obtained by Computer Simulation. Journal of Physical Chemistry B, 2011, 115, 3522-3530.	2.6	9
23	Simultaneous Application of the Gradient Theory and Monte Carlo Molecular Simulation for the Investigation of Methane/Water Interfacial Properties. Journal of Physical Chemistry B, 2011, 115, 9618-9625.	2.6	106
24	An Examination of the Ternary Methane + Carbon Dioxide + Water Phase Diagram using the SAFT-VR Approach. Journal of Physical Chemistry B, 2011, 115, 9604-9617.	2.6	30
25	Calculation of interfacial properties using molecular simulation with the reaction field method: Results for different water models. Journal of Chemical Physics, 2010, 132, .	3.0	35