Jean-FranÃ§ois DufrÃªche

List of Publications by Year
in descending order

69 papers	1,470 citations	236925 25 h-index	377865 34 g-index
69 all docs	69 docs citations	69 times ranked	1399 citing authors

#	Article	IF	Citations
1	How Acidity Rules Synergism and Antagonism in Liquidâ€“Liquid Extraction by Lipophilic Extractantsâ€”Part I: Determination of Nanostructures and Free Energies of Transfer. Solvent Extraction and Ion Exchange, 2022, 40, 86-105.	2.0	5
2	Molecular dynamics simulations of Eu(NO3)3 salt with DMDOHEMA in n-alkanes: Unravelling curvature properties in liquid-liquid extraction. Journal of Molecular Liquids, 2022, 348, 118035.	4.9	4
3	Effect of alkyl chains configurations of tertiary amines on uranium extraction and phase stability - Part II: curvature free energy controlling the ion transfer. Journal of Molecular Liquids, 2022, 349, 118487.	4.9	3
4	Experimentally probing ionic solutions in single-digit nanoconfinement. Journal of Colloid and Interface Science, 2022, 614, 396-404.	9.4	2
5	How Temperature Rise Can Induce Phase Separation in Aqueous Biphasic Solutions. Journal of Physical Chemistry Letters, 2022, 13, 2731-2736.	4.6	2
6	Why Local and Non-local Terms are Essential for Second Harmonic Generation Simulation?. Physical Chemistry Chemical Physics, 2022, , .	2.8	3
7	Electrostatic interactions in water: a nonlocal electrostatic approach. Molecular Physics, 2021, 119, e1825849.	1.7	8
8	Liquid/liquid interface in periodic boundary condition. Physical Chemistry Chemical Physics, 2021, 23, 1178-1187.	2.8	4
9	Experimental and Theoretical Study of Morphological and Charging Properties of Truncated Octahedron and Cubic Ceria Nanoparticles: Implications for Biomedical Applications. ACS Applied Nano Materials, 2021, 4, 1434-1444.	5.0	9
10	Phase separation of binary mixtures induced by soft centrifugal fields. Physical Chemistry Chemical Physics, 2021, 23, 8261-8272.	2.8	9
11	Thermodynamics of Malonamide Aggregation Deduced from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2021, 125, 3409-3418.	2.6	8
12	Molecular Forces in Liquidâ€“Liquid Extraction. Langmuir, 2021, 37, 10637-10656.	3.5	27
13	How Ion Pair Formation Drives Adsorption in the Electrical Double Layer: Molecular Dynamics of Charged Silicaâ€“Water Interfaces in the Presence of Divalent Alkaline Earth Ions. Journal of Physical Chemistry C, 2021, 125, 20551-20569.	3.1	5
14	Theory of Ternary Fluids under Centrifugal Fields. Journal of Physical Chemistry B, 2021, 125, 12054-12062.	2.6	5
15	Deciphering second harmonic generation signals. Chemical Science, 2021, 12, 15134-15142.	7.4	7
16	How Adsorption of Pheromones on Aerosols Controls Their Transport. ACS Central Science, 2020, 6, 1628-1638.	11.3	4
17	A thermodynamic model of non-ionic surfactants' micellization in the presence of polyoxometalates. Journal of Molecular Liquids, 2019, 293, 111280.	4.9	8
18	Synergistic Solvent Extraction Is Driven by Entropy. ACS Nano, 2019, 13, 13745-13758.	14.6	48

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19	Colloidal Model for the Prediction of the Extraction of Rare Earths Assisted by the Acidic Extractant. Langmuir, 2019, 35, 3215-3230.	3.5	29
20	Preferential Adsorption in Mixed Electrolytes Confined by Charged Amorphous Silica. Journal of Physical Chemistry C, 2019, 123, 16711-16720.	3.1	31
21	Investigation of the Structure of Concentrated NaOH Aqueous Solutions by Combining Molecular Dynamics and Wide-Angle X-ray Scattering. Journal of Physical Chemistry B, 2019, 123, 5121-5130.	2.6	11
22	Charge Properties of TiO₂ Nanotubes in NaNO₃ Aqueous Solution. ACS Applied Materials & Interfaces, 2018, 10, 13130-13142.	8.0	15
23	Non-additivity of ionic radii in electrolyte solutions: Hofmeister effect on mixtures modeled by an Associated MSA model. Journal of Molecular Liquids, 2018, 270, 30-39.	4.9	10
24	Molecular simulation of binary phase diagrams from the osmotic equilibrium method: vapour pressure and activity in waterâ€“ethanol mixtures. Molecular Physics, 2018, 116, 2009-2021.	1.7	9
25	Combined supramolecular and mesoscale modelling of liquidâ€“liquid extraction of rare earth salts. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2018, 555, 713-727.	4.7	18
26	Activity Coefficients of Aqueous Sodium, Calcium, and Europium Nitrate Solutions from Osmotic Equilibrium MD Simulations. Journal of Physical Chemistry B, 2018, 122, 7726-7736.	2.6	6
27	Measuring surface charge: Why experimental characterization and molecular modeling should be coupled. Current Opinion in Colloid and Interface Science, 2018, 37, 101-114.	7.4	39
28	Multicomponent Model for the Prediction of Nuclear Waste/Rare-Earth Extraction Processes. Langmuir, 2018, 34, 10434-10447.	3.5	22
29	Stability of reverse micelles in rare-earth separation: a chemical model based on a molecular approach. Physical Chemistry Chemical Physics, 2017, 19, 7094-7100.	2.8	24
30	Analysis of the second harmonic generation signal from a liquid/air and liquid/liquid interface. Journal of Chemical Physics, 2017, 146, 144701.	3.0	7
31	Scrutinizing Electro-Osmosis and Surface Conductivity with Molecular Dynamics. Journal of Physical Chemistry C, 2017, 121, 6756-6769.	3.1	28
32	Simulating Osmotic Equilibria: A New Tool for Calculating Activity Coefficients in Concentrated Aqueous Salt Solutions. Journal of Physical Chemistry B, 2017, 121, 9647-9658.	2.6	5
33	The role of curvature effects in liquidâ€“liquid extraction: assessing organic phase mesoscopic properties from MD simulations. Soft Matter, 2017, 13, 5518-5526.	2.7	22
34	Solvent Extraction: Structure of the Liquidâ€“Liquid Interface Containing a Diamide Ligand. Angewandte Chemie - International Edition, 2016, 55, 9326-9330.	13.8	53
35	A predictive model of reverse micelles solubilizing water for solvent extraction. Journal of Colloid and Interface Science, 2016, 479, 106-114.	9.4	23
36	Modeling and Speciation Study of Uranium(VI) and Technetium(VII) Coextraction with DEHiBA. Inorganic Chemistry, 2016, 55, 6511-6519.	4.0	29

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37	Modeling the transport of water and ionic tracers in a micrometric clay sample. Applied Clay Science, 2016, 123, 18-28.	5.2	14
38	How Ion Condensation Occurs at a Charged Surface: A Molecular Dynamics Investigation of the Stern Layer for Waterâ€“Silica Interfaces. Journal of Physical Chemistry C, 2016, 120, 963-973.	3.1	47
39	Thermodynamics of Associated Electrolytes in Water: Molecular Dynamics Simulations of Sulfate Solutions. Journal of Physical Chemistry B, 2015, 119, 11184-11195.	2.6	26
40	Recycling metals by controlled transfer of ionic species between complex fluids: en route to â€œienaicsâ€• Colloid and Polymer Science, 2015, 293, 1-22.	2.1	70
41	Ion-specific adsorption and electroosmosis in charged amorphous porous silica. Physical Chemistry Chemical Physics, 2015, 17, 24683-24695.	2.8	60
42	Strontium selectivity in sodium nonatitanate Na4Ti9O20Â·xH2O. Journal of Hazardous Materials, 2015, 283, 432-438.	12.4	31
43	Reverse aggregate nucleation induced by acids in liquidâ€“liquid extraction processes. Physical Chemistry Chemical Physics, 2014, 16, 7339.	2.8	47
44	Liquid-Liquid Extraction of Acids by a Malonamide: II-Anion Specific Effects in the Aggregate-Enhanced Extraction Isotherms. Solvent Extraction and Ion Exchange, 2014, 32, 620-636.	2.0	18
45	Predicting for thermodynamic instabilities in water/oil/surfactant microemulsions: A mesoscopic modelling approach. Journal of Chemical Physics, 2014, 140, 164711.	3.0	20
46	Role of non-ideality for the ion transport in porous media: Derivation of the macroscopic equations using upscaling. Physica D: Nonlinear Phenomena, 2014, 282, 39-60.	2.8	15
47	Mesoscopic modelling of frustration in microemulsions. Physical Chemistry Chemical Physics, 2013, 15, 7133.	2.8	35
48	Surfactant transfer across a water/oil interface: A diffusion/kinetics model for the interfacial tension evolution. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2013, 436, 1103-1110.	4.7	16
49	Ion transport in porous media: derivation of the macroscopic equations using upscaling and properties of the effective coefficients. Computational Geosciences, 2013, 17, 479-495.	2.4	31
50	How Do Anions Affect Self-Assembly and Solubility of Cetylpyridinium Surfactants in Water. Journal of Physical Chemistry B, 2013, 117, 1345-1356.	2.6	27
51	Recycling of Uranyl from Contaminated Water. Journal of Physical Chemistry B, 2013, 117, 10846-10851.	2.6	9
52	Asymptotic analysis of the Poissonâ€“Boltzmann equation describing electrokinetics in porous media. Nonlinearity, 2013, 26, 881-910.	1.4	12
53	Reverse Aggregates as Adaptive Selfâ€Assembled Systems for Selective Liquidâ€Liquid Cation Extraction. Israel Journal of Chemistry, 2013, 53, 108-112.	2.3	25
54	Nonequilibrium Vibrational Excitation of OH Radicals Generated During Multibubble Cavitation in Water. Journal of Physical Chemistry A, 2012, 116, 4860-4867.	2.5	50

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55	Kinetics of Triton-X100 Transfer Across the Water/Dodecane Interface: Analysis of the Interfacial Tension Variation. Journal of Physical Chemistry C, 2012, 116, 13152-13160.	3.1	23
56	Hydrophobic Transition in Porous Amorphous Silica. Journal of Physical Chemistry B, 2011, 115, 7881-7886.	2.6	57
57	Atomistic Description of Binary Lanthanoid Salt Solutions: A Coarse-Graining Approach. Journal of Physical Chemistry B, 2011, 115, 4329-4340.	2.6	14
58	Primitive models of ions in solution from molecular descriptions: A perturbation approach. Journal of Chemical Physics, 2011, 135, 234509.	3.0	28
59	Coarse-grained lanthanoid chloride aqueous solutions. Journal of Molecular Liquids, 2010, 153, 107-111.	4.9	6
60	Bridging molecular and continuous descriptions: the case of dynamics in clays. Anais Da Academia Brasileira De Ciencias, 2010, 82, 61-68.	0.8	8
61	Models of electrolyte solutions from molecular descriptions: The example of NaCl solutions. Physical Review E, 2009, 80, 065103.	2.1	27
62	Fluorescence Confocal Laser Scanning Microscopy for pH Mapping in a Coaxial Flow Microreactor: Application in the Synthesis of Superparamagnetic Nanoparticles. Journal of Physical Chemistry C, 2009, 113, 18097-18105.	3.1	35
63	Salt exclusion in charged porous media: a coarse-graining strategy in the case of montmorillonite clays. Physical Chemistry Chemical Physics, 2009, 11, 2023.	2.8	45
64	New coarse-graining procedure for the dynamics of charged spherical nanoparticles in solution. Journal of Chemical Physics, 2007, 126, 114108.	3.0	17
65	Modelling water and ion diffusion in clays: A multiscale approach. Comptes Rendus Chimie, 2007, 10, 1108-1116.	0.5	43
66	A multiscale approach to ion diffusion in clays: Building a two-state diffusionâ€“reaction scheme from microscopic dynamics. Journal of Colloid and Interface Science, 2007, 309, 289-295.	9.4	31
67	Lanthanide Salts Solutions:â€‰ Representation of Osmotic Coefficients within the Binding Mean Spherical Approximation. Journal of Physical Chemistry B, 2005, 109, 5243-5248.	2.6	34
68	How acidity rules synergism and antagonism in liquidâ€“liquid extraction by lipophilic extractantsâ€”Part II: application of the ienaic modelling. Solvent Extraction and Ion Exchange, 0, , 1-34.	2.0	3
69	Microemulsion as Model to Predict Free Energy of Transfer of Electrolyte in Solvent Extraction. Solvent Extraction and Ion Exchange, 0, , 1-36.	2.0	4