Eudes Eterno Fileti

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1792589/publications.pdf

Version: 2024-02-01

88 papers	1,932 citations	201575 27 h-index	330025 37 g-index
88 all docs	88 docs citations	88 times ranked	2220 citing authors

#	Article	IF	Citations
1	Effect of conductivity, viscosity, and density of water-in-salt electrolytes on the electrochemical behavior of supercapacitors: molecular dynamics simulations and in situ characterization studies. Materials Advances, 2022, 3, 611-623.	2.6	23
2	An evaluation of the capacitive behavior of supercapacitors as a function of the radius of cations using simulations with a constant potential method. Physical Chemistry Chemical Physics, 2022, 24, 3280-3288.	1.3	3
3	A molecular dynamics study of graphyne-based electrode and biocompatible ionic liquid for supercapacitor applications. Journal of Molecular Liquids, 2022, 360, 119494.	2.3	9
4	Combined Density Functional Theory and Molecular Dynamics Simulations To Investigate the Effects of Quantum and Double-Layer Capacitances in Functionalized Graphene as the Electrode Material of Aqueous-Based Supercapacitors. Journal of Physical Chemistry C, 2021, 125, 5518-5524.	1.5	12
5	Comparing Graphite and Graphene Oxide Supercapacitors with a Constant Potential Model. Journal of Physical Chemistry C, 2021, 125, 2318-2326.	1.5	13
6	Salt-in-water and water-in-salt electrolytes: the effects of the asymmetry in cation and anion valence on their properties. Physical Chemistry Chemical Physics, 2021, 24, 336-346.	1.3	8
7	Electric double layer formation and storing energy processes on graphene-based supercapacitors from electrical and thermodynamic perspectives. Journal of Molecular Modeling, 2020, 26, 159.	0.8	11
8	Computational Study of the Properties of Acetonitrile/Water-in-Salt Hybrid Electrolytes as Electrolytes for Supercapacitors. Journal of Physical Chemistry B, 2020, 124, 5685-5695.	1.2	13
9	Exploring doped or vacancy-modified graphene-based electrodes for applications in asymmetric supercapacitors. Physical Chemistry Chemical Physics, 2020, 22, 3906-3913.	1.3	26
10	An atomistic physico-chemical description of acetonitrile/tricyanomethanide based electrolytes. Journal of Molecular Liquids, 2019, 292, 111439.	2.3	4
11	Investigating the asymmetry in the EDL response of C₆₀/graphene supercapacitors. Physical Chemistry Chemical Physics, 2019, 21, 15362-15371.	1.3	17
12	Atomistic study of the physical properties of sulfonium-based ionic liquids as electrolyte for supercapacitors. Journal of Molecular Liquids, 2019, 296, 112065.	2.3	19
13	Impact of Edge Groups on the Hydration and Aggregation Properties of Graphene Oxide. Journal of Physical Chemistry B, 2018, 122, 2578-2586.	1.2	15
14	Elucidating the amphiphilic character of graphene oxide. Physical Chemistry Chemical Physics, 2018, 20, 9507-9515.	1.3	40
15	Graphene/ionic liquid ultracapacitors: does ionic size correlate with energy storage performance?. New Journal of Chemistry, 2018, 42, 18409-18417.	1.4	26
16	Storing Energy in Biodegradable Electrochemical Supercapacitors. ACS Omega, 2018, 3, 13869-13875.	1.6	46
17	Differential Capacitance and Energetics of the Electrical Double Layer of Graphene Oxide Supercapacitors: Impact of the Oxidation Degree. Journal of Physical Chemistry C, 2018, 122, 21824-21832.	1.5	30
18	GIAO-DFT-NMR characterization of fullerene-cucurbituril complex: the effects of the C60@CB[9] host-guest mutual interactions. Journal of Molecular Modeling, 2018, 24, 181.	0.8	5

#	Article	IF	Citations
19	All-boron fullerene exhibits a strong affinity to inorganic anions. Chemical Physics Letters, 2017, 671, 107-112.	1.2	6
20	Imidazolium Ionic Liquid Mediates Black Phosphorus Exfoliation while Preventing Phosphorene Decomposition. ACS Nano, 2017, 11, 6459-6466.	7.3	43
21	Solubility origin at the nanoscale: enthalpic and entropic contributions in polar and nonpolar environments. Physical Chemistry Chemical Physics, 2017, 19, 3903-3910.	1.3	6
22	Exfoliation of Graphene in Ionic Liquids: Pyridinium versus Pyrrolidinium. Journal of Physical Chemistry C, 2017, 121, 911-917.	1.5	30
23	Hydration properties of the polyalanines by atomistic molecular dynamics. Journal of Molecular Liquids, 2017, 244, 285-290.	2.3	6
24	Assessing the interaction between surfactant-like peptides and lipid membranes. RSC Advances, 2017, 7, 35973-35981.	1.7	22
25	Elucidating the stability of bolaamphiphilic polypeptide nanosheets using atomistic molecular dynamics. Physical Chemistry Chemical Physics, 2017, 19, 31921-31928.	1.3	26
26	Hydration peculiarities of graphene oxides with multiple oxidation degrees. Physical Chemistry Chemical Physics, 2017, 19, 32333-32340.	1.3	21
27	Which fullerenols are water soluble? Systematic atomistic investigation. New Journal of Chemistry, 2017, 41, 184-189.	1.4	16
28	Potential energy surface of excited semiconductors: Graphene quantum dot and BODIPY. Chemical Physics, 2016, 474, 1-6.	0.9	9
29	Atomically precise understanding of nanofluids: nanodiamonds and carbon nanotubes in ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 26865-26872.	1.3	10
30	Versatile interactions of boron fullerene B₈₀with gas molecules. RSC Advances, 2016, 6, 78684-78691.	1.7	4
31	Peculiar Aqueous Solubility Trend in Cucurbiturils Unraveled by Atomistic Simulations. Journal of Physical Chemistry B, 2016, 120, 7511-7516.	1.2	11
32	Protein remains stable at unusually high temperatures when solvated in aqueous mixtures of amino acid based ionic liquids. Journal of Molecular Modeling, 2016, 22, 258.	0.8	14
33	Free energy of solvation of carbon nanotubes in pyridinium-based ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 20357-20362.	1.3	7
34	Ionization of cucurbiturils as a pathway to more stable hostâ€“guest complexes. Computational and Theoretical Chemistry, 2016, 1083, 7-11.	1.1	4
35	Selfâ€Assembled Peptideâ€“Polyfluorene Nanocomposites for Biodegradable Organic Electronics. Advanced Materials Interfaces, 2015, 2, 1500265.	1.9	35
36	Enhanced stability of the model miniâ€protein in amino acid ionic liquids and their aqueous solutions. Journal of Computational Chemistry, 2015, 36, 2044-2051.	1.5	35

#	Article	IF	Citations
37	Strong electronic polarization of the C₆₀ fullerene by imidazolium-based ionic liquids: accurate insights from Bornâ€“Oppenheimer molecular dynamic simulations. Physical Chemistry Chemical Physics, 2015, 17, 15739-15745.	1.3	18
38	Can inorganic salts tune electronic properties of graphene quantum dots?. Physical Chemistry Chemical Physics, 2015, 17, 17413-17420.	1.3	29
39	The force field for imidazolium-based ionic liquids: Novel anions with polar residues. Chemical Physics Letters, 2015, 633, 132-138.	1.2	13
40	Ionic Clusters vs Shear Viscosity in Aqueous Amino Acid Ionic Liquids. Journal of Physical Chemistry B, 2015, 119, 3824-3828.	1.2	23
41	The Band Gap of Graphene Is Efficiently Tuned by Monovalent Ions. Journal of Physical Chemistry Letters, 2015, 6, 302-307.	2.1	50
42	Buckybomb: Reactive Molecular Dynamics Simulation. Journal of Physical Chemistry Letters, 2015, 6, 913-917.	2.1	31
43	Mixtures of amino-acid based ionic liquids and water. Journal of Molecular Modeling, 2015, 21, 236.	0.8	17
44	Polypeptide A9K at nanoscale carbon: a simulation study. Physical Chemistry Chemical Physics, 2015, 17, 26386-26393.	1.3	4
45	Graphene exfoliation in ionic liquids: unified methodology. RSC Advances, 2015, 5, 81229-81234.	1.7	26
46	Imidazolium Ionic Liquid Helps to Disperse Fullerenes in Water. Journal of Physical Chemistry Letters, 2014, 5, 1795-1800.	2.1	38
47	The role of water and structure on the generation of reactive oxygen species in peptide/hypericin complexes. Journal of Peptide Science, 2014, 20, 554-562.	0.8	22
48	The scaled-charge additive force field for amino acid based ionic liquids. Chemical Physics Letters, 2014, 616-617, 205-211.	1.2	41
49	Molecular Dynamics Study of Surfactant-Like Peptide Based Nanostructures. Journal of Physical Chemistry B, 2014, 118, 12215-12222.	1.2	49
50	Assessing the hydration free energy of a homologous series of polyols with classical and quantum mechanical solvation models. Physical Chemistry Chemical Physics, 2014, 16, 17863-17868.	1.3	2
51	Solvent Polarity Considerations Are Unable to Describe Fullerene Solvation Behavior. Journal of Physical Chemistry B, 2014, 118, 3378-3384.	1.2	25
52	Atomistic Description of Fullerene-Based Membranes. Journal of Physical Chemistry B, 2014, 118, 12471-12477.	1.2	6
53	Molecular Description of Surfactant-like Peptide Based Membranes. Journal of Physical Chemistry C, 2014, 118, 9598-9603.	1.5	29
54	Predicting the properties of a new class of hostâ€“guest complexes: C₆₀ fullerene and CB[9] cucurbituril. Physical Chemistry Chemical Physics, 2014, 16, 22823-22829.	1.3	20

#	Article	IF	Citations
55	Exploding Nitromethane in Silico, in Real Time. Journal of Physical Chemistry Letters, 2014, 5, 3415-3420.	2.1	17
56	Does the Like Dissolves Like Rule Hold for Fullerene and Ionic Liquids?. Journal of Solution Chemistry, 2014, 43, 1019-1031.	0.6	40
57	Structure and Supersaturation of Highly Concentrated Solutions of Buckyball in 1-Butyl-3-Methylimidazolium Tetrafluoroborate. Journal of Physical Chemistry B, 2014, 118, 7376-7382.	1.2	12
58	Ab initio study of weakly bound halogen complexes: RXâ‹¯PH3. Journal of Molecular Modeling, 2013, 19, 329-336.	0.8	15
59	Structural and Photophysical Properties of Peptide Micro/Nanotubes Functionalized with Hypericin. Journal of Physical Chemistry B, 2013, 117, 2605-2614.	1.2	35
60	Molecular interactions between fullerene C60 and ionic liquids. Chemical Physics Letters, 2013, 568-569, 75-79.	1.2	35
61	Prediction of the Hydration Properties of Diamondoids from Free Energy and Potential of Mean Force Calculations. Journal of Physical Chemistry B, 2012, 116, 13467-13471.	1.2	8
62	Influence of pH and Pyrenyl on the Structural and Morphological Control of Peptide Nanotubes. Journal of Physical Chemistry C, 2011, 115, 7906-7913.	1.5	23
63	Effect of solute flexibility and polarization on the solvatochromic shift of a brominated merocyanine dye in water: A sequential MD/QM study. International Journal of Quantum Chemistry, 2011, 111, 1607-1615.	1.0	6
64	Gasâ€phase acylium ion transfer reactions mediated by a proton shuttle mechanism. International Journal of Quantum Chemistry, 2011, 111, 1596-1606.	1.0	6
65	Theoretical analysis of the hydration of C60 in normal and supercritical conditions. Carbon, 2011, 49, 187-192.	5.4	29
66	Assessing the solvation mechanism of C60(OH)24 in aqueous solution. Chemical Physics Letters, 2011, 507, 244-247.	1.2	34
67	Molecular dynamics simulation of liquid trimethylphosphine. Journal of Chemical Physics, 2011, 135, 064506.	1.2	3
68	Hyperpolarizabilities of the methanol molecule: A CCSD calculation including vibrational corrections. Journal of Chemical Physics, 2010, 132, 034307.	1.2	26
69	Liquid separation by a graphene membrane. Journal of Applied Physics, 2010, 108, 113527.	1.1	14
70	Ab initio analysis of monomers and dimers of trialkylphosphine oxides: Structural and thermodynamic stability. International Journal of Quantum Chemistry, 2009, 109, 250-258.	1.0	4
71	The 13C NMR properties of low hydroxylated fullerenes with density functional theory. Chemical Physics Letters, 2009, 467, 339-343.	1.2	21
72	Note on the Free Energy of Transfer of Fullerene C₆₀ Simulated by Using Classical Potentials. Journal of Physical Chemistry B, 2009, 113, 7045-7048.	1.2	33

#	Article	IF	Citations
73	Structure, stability, depolarized light scattering, and vibrational spectra of fullerenols from all-electron density-functional-theory calculations. Physical Review A, 2009, 79, .	1.0	30
74	Calculations of vibrational frequencies, Raman activities and degrees of depolarization for complexes involving water, methanol and ethanol. Chemical Physics Letters, 2008, 452, 54-58.	1.2	31
75	Effects of hydroxyl group distribution on the reactivity, stability and optical properties of fullerenols. Nanotechnology, 2008, 19, 365703.	1.3	36
76	Effects of hydroxyl group distribution on the reactivity, stability and optical properties of fullerenols. Nanotechnology, 2008, 19, 509801-289801.	1.3	2
77	Structure and UVâˆ'Vis Spectrum of C₆₀ Fullerene in Ethanol:â€‰ A Sequential Molecular Dynamics/Quantum Mechanics Study. Journal of Physical Chemistry B, 2007, 111, 11935-11939.	1.2	40
78	Isotropic and anisotropic NMR chemical shifts in liquid water: a sequential QM/MM study. Journal of the Brazilian Chemical Society, 2007, 18, 74-84.	0.6	24
79	Gasâ€phase electrophilic addition promoted by CH₃S⁺ï£¾ CH₂ ions on aromatic systems. Journal of Mass Spectrometry, 2007, 42, 1310-1318.	0.7	8
80	Ab Initio Study of the Isomeric Equilibrium of the HCNÂ·Â·Â·H2O and H2OÂ·Â·Â·HCN Hydrogen-Bonded Clusters. Journal of Physical Chemistry A, 2006, 110, 10303-10308.	1.1	27
81	Ab initio NMR study of the isomeric hydrogen-bonded methanol-water complexes. International Journal of Quantum Chemistry, 2005, 102, 554-564.	1.0	15
82	Calculated infrared spectra of hydrogen-bonded methanol-water, water-methanol, and methanol-methanol complexes. International Journal of Quantum Chemistry, 2005, 104, 808-815.	1.0	34
83	A sequential Monte Carlo/Quantum Mechanics study of the dipole polarizability of liquid benzene. Journal of Computational Methods in Sciences and Engineering, 2004, 4, 559-568.	0.1	2
84	Is There a Favorite Isomer for Hydrogen-Bonded Methanol in Water?. Advances in Quantum Chemistry, 2004, 47, 51-63.	0.4	12
85	Relative strength of hydrogen bond interaction in alcoholâ€"water complexes. Chemical Physics Letters, 2004, 400, 494-499.	1.2	135
86	Rayleigh and Raman light scattering in hydrogen-bonded acetonitrile?water. Theoretical Chemistry Accounts, 2003, 110, 360-366.	0.5	18
87	Electronic changes due to thermal disorder of hydrogen bonds in liquids: Pyridine in an aqueous environment. Physical Review E, 2003, 67, 061504.	0.8	48
88	Rayleigh light scattering of hydrogen bonded clusters investigated by means ofab initiocalculations. Journal of Physics B: Atomic, Molecular and Optical Physics, 2003, 36, 399-408.	0.6	41