

Eudes Eterno Fileti

List of Publications by Year in descending order

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88
papers

1,932
citations

201385

27
h-index

329751

37
g-index

88
all docs

88
docs citations

88
times ranked

2220
citing authors

#	ARTICLE	IF	CITATIONS
1	Relative strength of hydrogen bond interaction in alcohol-water complexes. <i>Chemical Physics Letters</i> , 2004, 400, 494-499.	1.2	135
2	The Band Gap of Graphene Is Efficiently Tuned by Monovalent Ions. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 302-307.	2.1	50
3	Molecular Dynamics Study of Surfactant-Like Peptide Based Nanostructures. <i>Journal of Physical Chemistry B</i> , 2014, 118, 12215-12222.	1.2	49
4	Electronic changes due to thermal disorder of hydrogen bonds in liquids: Pyridine in an aqueous environment. <i>Physical Review E</i> , 2003, 67, 061504.	0.8	48
5	Storing Energy in Biodegradable Electrochemical Supercapacitors. <i>ACS Omega</i> , 2018, 3, 13869-13875.	1.6	46
6	Imidazolium Ionic Liquid Mediates Black Phosphorus Exfoliation while Preventing Phosphorene Decomposition. <i>ACS Nano</i> , 2017, 11, 6459-6466.	7.3	43
7	Rayleigh light scattering of hydrogen bonded clusters investigated by means of ab initio calculations. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2003, 36, 399-408.	0.6	41
8	The scaled-charge additive force field for amino acid based ionic liquids. <i>Chemical Physics Letters</i> , 2014, 616-617, 205-211.	1.2	41
9	Structure and UV-Vis Spectrum of C ₆₀ Fullerene in Ethanol: A Sequential Molecular Dynamics/Quantum Mechanics Study. <i>Journal of Physical Chemistry B</i> , 2007, 111, 11935-11939.	1.2	40
10	Does the Like Dissolves Like Rule Hold for Fullerene and Ionic Liquids?. <i>Journal of Solution Chemistry</i> , 2014, 43, 1019-1031.	0.6	40
11	Elucidating the amphiphilic character of graphene oxide. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 9507-9515.	1.3	40
12	Imidazolium Ionic Liquid Helps to Disperse Fullerenes in Water. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1795-1800.	2.1	38
13	Effects of hydroxyl group distribution on the reactivity, stability and optical properties of fullerenols. <i>Nanotechnology</i> , 2008, 19, 365703.	1.3	36
14	Structural and Photophysical Properties of Peptide Micro/Nanotubes Functionalized with Hypericin. <i>Journal of Physical Chemistry B</i> , 2013, 117, 2605-2614.	1.2	35
15	Molecular interactions between fullerene C ₆₀ and ionic liquids. <i>Chemical Physics Letters</i> , 2013, 568-569, 75-79.	1.2	35
16	Self-Assembled Peptide-Polyfluorene Nanocomposites for Biodegradable Organic Electronics. <i>Advanced Materials Interfaces</i> , 2015, 2, 1500265.	1.9	35
17	Enhanced stability of the model mini-protein in amino acid ionic liquids and their aqueous solutions. <i>Journal of Computational Chemistry</i> , 2015, 36, 2044-2051.	1.5	35
18	Calculated infrared spectra of hydrogen-bonded methanol-water, water-methanol, and methanol-methanol complexes. <i>International Journal of Quantum Chemistry</i> , 2005, 104, 808-815.	1.0	34

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19	Assessing the solvation mechanism of C ₆₀ (OH) ₂₄ in aqueous solution. <i>Chemical Physics Letters</i> , 2011, 507, 244-247.	1.2	34
20	Note on the Free Energy of Transfer of Fullerene C ₆₀ Simulated by Using Classical Potentials. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7045-7048.	1.2	33
21	Calculations of vibrational frequencies, Raman activities and degrees of depolarization for complexes involving water, methanol and ethanol. <i>Chemical Physics Letters</i> , 2008, 452, 54-58.	1.2	31
22	Buckybomb: Reactive Molecular Dynamics Simulation. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 913-917.	2.1	31
23	Structure, stability, depolarized light scattering, and vibrational spectra of fullerenols from all-electron density-functional-theory calculations. <i>Physical Review A</i> , 2009, 79, .	1.0	30
24	Exfoliation of Graphene in Ionic Liquids: Pyridinium versus Pyrrolidinium. <i>Journal of Physical Chemistry C</i> , 2017, 121, 911-917.	1.5	30
25	Differential Capacitance and Energetics of the Electrical Double Layer of Graphene Oxide Supercapacitors: Impact of the Oxidation Degree. <i>Journal of Physical Chemistry C</i> , 2018, 122, 21824-21832.	1.5	30
26	Theoretical analysis of the hydration of C ₆₀ in normal and supercritical conditions. <i>Carbon</i> , 2011, 49, 187-192.	5.4	29
27	Molecular Description of Surfactant-like Peptide Based Membranes. <i>Journal of Physical Chemistry C</i> , 2014, 118, 9598-9603.	1.5	29
28	Can inorganic salts tune electronic properties of graphene quantum dots?. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 17413-17420.	1.3	29
29	Ab Initio Study of the Isomeric Equilibrium of the HCN⋯H ₂ O and H ₂ O⋯HCN Hydrogen-Bonded Clusters. <i>Journal of Physical Chemistry A</i> , 2006, 110, 10303-10308.	1.1	27
30	Hyperpolarizabilities of the methanol molecule: A CCSD calculation including vibrational corrections. <i>Journal of Chemical Physics</i> , 2010, 132, 034307.	1.2	26
31	Graphene exfoliation in ionic liquids: unified methodology. <i>RSC Advances</i> , 2015, 5, 81229-81234.	1.7	26
32	Elucidating the stability of bolaamphiphilic polypeptide nanosheets using atomistic molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 31921-31928.	1.3	26
33	Graphene/ionic liquid ultracapacitors: does ionic size correlate with energy storage performance?. <i>New Journal of Chemistry</i> , 2018, 42, 18409-18417.	1.4	26
34	Exploring doped or vacancy-modified graphene-based electrodes for applications in asymmetric supercapacitors. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 3906-3913.	1.3	26
35	Solvent Polarity Considerations Are Unable to Describe Fullerene Solvation Behavior. <i>Journal of Physical Chemistry B</i> , 2014, 118, 3378-3384.	1.2	25
36	Isotropic and anisotropic NMR chemical shifts in liquid water: a sequential QM/MM study. <i>Journal of the Brazilian Chemical Society</i> , 2007, 18, 74-84.	0.6	24

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37	Influence of pH and Pyrenyl on the Structural and Morphological Control of Peptide Nanotubes. <i>Journal of Physical Chemistry C</i> , 2011, 115, 7906-7913.	1.5	23
38	Ionic Clusters vs Shear Viscosity in Aqueous Amino Acid Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2015, 119, 3824-3828.	1.2	23
39	Effect of conductivity, viscosity, and density of water-in-salt electrolytes on the electrochemical behavior of supercapacitors: molecular dynamics simulations and <i>in situ</i> characterization studies. <i>Materials Advances</i> , 2022, 3, 611-623.	2.6	23
40	The role of water and structure on the generation of reactive oxygen species in peptide/hypericin complexes. <i>Journal of Peptide Science</i> , 2014, 20, 554-562.	0.8	22
41	Assessing the interaction between surfactant-like peptides and lipid membranes. <i>RSC Advances</i> , 2017, 7, 35973-35981.	1.7	22
42	The ¹³ C NMR properties of low hydroxylated fullerenes with density functional theory. <i>Chemical Physics Letters</i> , 2009, 467, 339-343.	1.2	21
43	Hydration peculiarities of graphene oxides with multiple oxidation degrees. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32333-32340.	1.3	21
44	Predicting the properties of a new class of host-guest complexes: C ₆₀ fullerene and CB[9] cucurbituril. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 22823-22829.	1.3	20
45	Atomistic study of the physical properties of sulfonium-based ionic liquids as electrolyte for supercapacitors. <i>Journal of Molecular Liquids</i> , 2019, 296, 112065.	2.3	19
46	Rayleigh and Raman light scattering in hydrogen-bonded acetonitrile/water. <i>Theoretical Chemistry Accounts</i> , 2003, 110, 360-366.	0.5	18
47	Strong electronic polarization of the C ₆₀ fullerene by imidazolium-based ionic liquids: accurate insights from Born-Oppenheimer molecular dynamic simulations. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 15739-15745.	1.3	18
48	Exploding Nitromethane in Silico, in Real Time. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3415-3420.	2.1	17
49	Mixtures of amino-acid based ionic liquids and water. <i>Journal of Molecular Modeling</i> , 2015, 21, 236.	0.8	17
50	Investigating the asymmetry in the EDL response of C ₆₀ /graphene supercapacitors. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 15362-15371.	1.3	17
51	Which fullerenols are water soluble? Systematic atomistic investigation. <i>New Journal of Chemistry</i> , 2017, 41, 184-189.	1.4	16
52	Ab initio NMR study of the isomeric hydrogen-bonded methanol-water complexes. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 554-564.	1.0	15
53	Ab initio study of weakly bound halogen complexes: RX ⁻ PH ₃ . <i>Journal of Molecular Modeling</i> , 2013, 19, 329-336.	0.8	15
54	Impact of Edge Groups on the Hydration and Aggregation Properties of Graphene Oxide. <i>Journal of Physical Chemistry B</i> , 2018, 122, 2578-2586.	1.2	15

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55	Liquid separation by a graphene membrane. <i>Journal of Applied Physics</i> , 2010, 108, 113527.	1.1	14
56	Protein remains stable at unusually high temperatures when solvated in aqueous mixtures of amino acid based ionic liquids. <i>Journal of Molecular Modeling</i> , 2016, 22, 258.	0.8	14
57	The force field for imidazolium-based ionic liquids: Novel anions with polar residues. <i>Chemical Physics Letters</i> , 2015, 633, 132-138.	1.2	13
58	Computational Study of the Properties of Acetonitrile/Water-in-Salt Hybrid Electrolytes as Electrolytes for Supercapacitors. <i>Journal of Physical Chemistry B</i> , 2020, 124, 5685-5695.	1.2	13
59	Comparing Graphite and Graphene Oxide Supercapacitors with a Constant Potential Model. <i>Journal of Physical Chemistry C</i> , 2021, 125, 2318-2326.	1.5	13
60	Is There a Favorite Isomer for Hydrogen-Bonded Methanol in Water?. <i>Advances in Quantum Chemistry</i> , 2004, 47, 51-63.	0.4	12
61	Structure and Supersaturation of Highly Concentrated Solutions of Buckyball in 1-Butyl-3-Methylimidazolium Tetrafluoroborate. <i>Journal of Physical Chemistry B</i> , 2014, 118, 7376-7382.	1.2	12
62	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. <i>Journal of Physical Chemistry C</i> , 2021, 125, 5518-5524.	1.5	12
63	Peculiar Aqueous Solubility Trend in Cucurbiturils Unraveled by Atomistic Simulations. <i>Journal of Physical Chemistry B</i> , 2016, 120, 7511-7516.	1.2	11
64	Electric double layer formation and storing energy processes on graphene-based supercapacitors from electrical and thermodynamic perspectives. <i>Journal of Molecular Modeling</i> , 2020, 26, 159.	0.8	11
65	Atomically precise understanding of nanofluids: nanodiamonds and carbon nanotubes in ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26865-26872.	1.3	10
66	Potential energy surface of excited semiconductors: Graphene quantum dot and BODIPY. <i>Chemical Physics</i> , 2016, 474, 1-6.	0.9	9
67	A molecular dynamics study of graphyne-based electrode and biocompatible ionic liquid for supercapacitor applications. <i>Journal of Molecular Liquids</i> , 2022, 360, 119494.	2.3	9
68	Gas-phase electrophilic addition promoted by $\text{CH}_3\text{S}^+\text{CH}_2$ ions on aromatic systems. <i>Journal of Mass Spectrometry</i> , 2007, 42, 1310-1318.	0.7	8
69	Prediction of the Hydration Properties of Diamondoids from Free Energy and Potential of Mean Force Calculations. <i>Journal of Physical Chemistry B</i> , 2012, 116, 13467-13471.	1.2	8
70	Salt-in-water and water-in-salt electrolytes: the effects of the asymmetry in cation and anion valence on their properties. <i>Physical Chemistry Chemical Physics</i> , 2021, 24, 336-346.	1.3	8
71	Free energy of solvation of carbon nanotubes in pyridinium-based ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20357-20362.	1.3	7
72	Effect of solute flexibility and polarization on the solvatochromic shift of a brominated merocyanine dye in water: A sequential MD/QM study. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1607-1615.	1.0	6

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73	Gas-phase acylium ion transfer reactions mediated by a proton shuttle mechanism. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1596-1606.	1.0	6
74	Atomistic Description of Fullerene-Based Membranes. <i>Journal of Physical Chemistry B</i> , 2014, 118, 12471-12477.	1.2	6
75	All-boron fullerene exhibits a strong affinity to inorganic anions. <i>Chemical Physics Letters</i> , 2017, 671, 107-112.	1.2	6
76	Solubility origin at the nanoscale: enthalpic and entropic contributions in polar and nonpolar environments. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3903-3910.	1.3	6
77	Hydration properties of the polyanilines by atomistic molecular dynamics. <i>Journal of Molecular Liquids</i> , 2017, 244, 285-290.	2.3	6
78	GIAO-DFT-NMR characterization of fullerene-cucurbituril complex: the effects of the C ₆₀ @CB[9] host-guest mutual interactions. <i>Journal of Molecular Modeling</i> , 2018, 24, 181.	0.8	5
79	Ab initio analysis of monomers and dimers of trialkylphosphine oxides: Structural and thermodynamic stability. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 250-258.	1.0	4
80	Polypeptide A9K at nanoscale carbon: a simulation study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 26386-26393.	1.3	4
81	Versatile interactions of boron fullerene B ₈₀ with gas molecules. <i>RSC Advances</i> , 2016, 6, 78684-78691.	1.7	4
82	Ionization of cucurbiturils as a pathway to more stable host-guest complexes. <i>Computational and Theoretical Chemistry</i> , 2016, 1083, 7-11.	1.1	4
83	An atomistic physico-chemical description of acetonitrile/tricyanomethanide based electrolytes. <i>Journal of Molecular Liquids</i> , 2019, 292, 111439.	2.3	4
84	Molecular dynamics simulation of liquid trimethylphosphine. <i>Journal of Chemical Physics</i> , 2011, 135, 064506.	1.2	3
85	An evaluation of the capacitive behavior of supercapacitors as a function of the radius of cations using simulations with a constant potential method. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 3280-3288.	1.3	3
86	A sequential Monte Carlo/Quantum Mechanics study of the dipole polarizability of liquid benzene. <i>Journal of Computational Methods in Sciences and Engineering</i> , 2004, 4, 559-568.	0.1	2
87	Effects of hydroxyl group distribution on the reactivity, stability and optical properties of fullerenols. <i>Nanotechnology</i> , 2008, 19, 509801-289801.	1.3	2
88	Assessing the hydration free energy of a homologous series of polyols with classical and quantum mechanical solvation models. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17863-17868.	1.3	2