Mehdi Shakourian-Fard

List of Publications by Year
in descending order

47 papers	987 citations	516710 16 h-index	454955 30 g-index
49 all docs	49 docs citations	49 times ranked	1368 citing authors

#	Article	IF	Citations
1	Trends in Na-Ion Solvation with Alkyl-Carbonate Electrolytes for Sodium-Ion Batteries: Insights from First-Principles Calculations. Journal of Physical Chemistry C, 2015, 119, 22747-22759.	3.1	84
2	In Silico Based Rank-Order Determination and Experiments on Nonaqueous Electrolytes for Sodium Ion Battery Applications. Journal of Physical Chemistry C, 2014, 118, 13406-13416.	3.1	74
3	Meta-Hybrid Density Functional Theory Study of Adsorption of Imidazolium- and Ammonium-Based Ionic Liquids on Graphene Sheet. Journal of Physical Chemistry C, 2015, 119, 7095-7108.	3.1	68
4	Design of silica supported task-specific ionic liquid catalyst system for oxidation of cyclohexene to adipic acid with 30% H2O2. Catalysis Communications, 2012, 26, 54-57.	3.3	60
5	Trends in Physisorption of Ionic Liquids on Boron-Nitride Sheets. Journal of Physical Chemistry C, 2014, 118, 26003-26016.	3.1	54
6	Selective oxidation of sulfides to sulfoxides by a molybdate-based catalyst using 30% hydrogen peroxide. Catalysis Communications, 2014, 52, 16-21.	3.3	46
7	Immobilizing magnetic glutaraldehyde cross-linked chitosan on graphene oxide and nitrogen-doped graphene oxide as well-dispersible adsorbents for chromate removal from aqueous solutions. International Journal of Biological Macromolecules, 2019, 128, 61-73.	7.5	43
8	A magnetic supported iron complex for selective oxidation of sulfides to sulfoxides using 30% hydrogen peroxide at room temperature. RSC Advances, 2014, 4, 44274-44281.	3.6	38
9	Silver nanoparticles supported on silica-coated ferrite as magnetic and reusable catalysts for oxidant-free alcohol dehydrogenation. RSC Advances, 2015, 5, 22503-22509.	3.6	38
10	Evaluating the Free Energies of Solvation and Electronic Structures of Lithiumâ€ion Battery Electrolytes. ChemPhysChem, 2016, 17, 2916-2930.	2.1	36
11	Ionic Liquid Based on Î±-Amino Acid Anion and N7,N9-Dimethylguaninium Cation ([dMG][AA]): Theoretical Study on the Structure and Electronic Properties. Journal of Physical Chemistry A, 2012, 116, 5436-5444.	2.5	30
12	The effect of defect types on the electronic and optical properties of graphene nanoflakes physisorbed by ionic liquids. Physical Chemistry Chemical Physics, 2017, 19, 4383-4395.	2.8	29
13	Calcium-Ion Batteries: Identifying Ideal Electrolytes for Next-Generation Energy Storage Using Computational Analysis. Journal of Physical Chemistry C, 2019, 123, 15885-15896.	3.1	29
14	Quantitative structure-property relationship for melting and freezing points of deep eutectic solvents. Journal of Molecular Liquids, 2021, 321, 114744.	4.9	26
15	Synthesis of Î±-Aminophosphonates in the Presence of a Magnetic Recyclable Fe3O4@SiO2-2mimSO3H Nanocatalyst. Bulletin of the Chemical Society of Japan, 2014, 87, 982-987.	3.2	22
16	Influence of the hydrogen bonding on the basicity of selected macrocyclic amines. Journal of Physical Organic Chemistry, 2012, 25, 803-810.	1.9	19
17	Effect of mono-vacant defects on the opto-electronic properties of ionic liquid functionalized hexagonal boron-nitride nanosheets. Journal of Molecular Liquids, 2018, 249, 1172-1182.	4.9	17
18	A green procedure for direct oxidation of organic halides to aldehydes and ketones catalyzed by a molybdate-based catalyst. New Journal of Chemistry, 2015, 39, 3845-3851.	2.8	16

#	Article	IF	Citations
19	A DFT study of the adsorption of deep eutectic solvents onto graphene and defective graphene nanoflakes. Journal of Molecular Liquids, 2021, 327, 114850.	4.9	16
20	Unraveling the effect of nitrogen doping on graphene nanoflakes and the adsorption properties of ionic liquids: A DFT study. Journal of Molecular Liquids, 2020, 312, 113400.	4.9	16
21	Electronic Structure Insights into the Solvation of Magnesium Ions with Cyclic and Acyclic Carbonates. ChemPhysChem, 2015, 16, 3607-3617.	2.1	15
22	The effect of ionic liquid adsorption on the electronic and optical properties of fluorographene nanosheets. Journal of Molecular Liquids, 2018, 268, 206-214.	4.9	15
23	The effect of sulfur and nitrogen/sulfur co-doping in graphene surface on the adsorption of toxic heavy metals (Cd, Hg, Pb). Journal of Materials Science, 2019, 54, 13175-13189.	3.7	14
24	Cooperativity effects of intramolecular OHâ€¦O interactions on pK _a values of polyolalkyl sulfonic acids in the gas phase and solution: a density functional theory study. Journal of Physical Organic Chemistry, 2014, 27, 604-612.	1.9	13
25	Molecular structure and character of bonding of mono and divalent metal cations (Li+, Na+, K+,) Tj ETQq1 1 0.784314 rgBT /Overlock 1 613-626.	2.0	12
26	A highly reactive and magnetic recyclable catalyst based on silver nanoparticles supported on ferrite for Nâ€monoalkylation of amines with alcohols. Applied Organometallic Chemistry, 2017, 31, e3720.	3.5	12
27	Theoretical investigation on the structural and electronic properties of complexes formed by thymine and 2â€²-deoxythymidine with different anions. Structural Chemistry, 2012, 23, 17-28.	2.0	11
28	Selective aqueous oxidation of alcohols catalyzed by copper (II) phthalocyanine nanoparticles. Comptes Rendus Chimie, 2016, 19, 314-319.	0.5	11
29	Defectâ€Based Modulation of Optoelectronic Properties for Biofunctionalized Hexagonal Boron Nitride Nanosheets. ChemPhysChem, 2017, 18, 2328-2335.	2.1	11
30	Tailoring of graphene quantum dots for toxic heavy metals detection. Applied Physics A: Materials Science and Processing, 2019, 125, 1.	2.3	11
31	Adsorption mechanism of toxic heavy metal ions on oxygen-passivated nanopores in graphene nanoflakes. Journal of Materials Science, 2020, 55, 15826-15844.	3.7	11
32	Density functional theory investigation into the interaction of deep eutectic solvents with amino acids. Journal of Molecular Liquids, 2021, 343, 117624.	4.9	11
33	Surface Chargeâ€Transfer Doping of Graphene Nanoflakes Containing Doubleâ€Vacancy (5â€8â€5) and Stoneâ€Wales (55â€77) Defects through Molecular Adsorption. ChemPhysChem, 2016, 17, 3289-3299.	2.1	10
34	Interaction of cations with 2â€²â€deoxythymidine nucleoside and analysis of the nature and strength of cation bonds. Journal of Physical Organic Chemistry, 2012, 25, 153-161.	1.9	9
35	Influence of the water molecules (nÂ=Â1â€“6) on the interaction between Li+, Na+, K+ cations and indole molecule as tryptophan amino acid residue. Structural Chemistry, 2012, 23, 857-865.	2.0	8
36	Silver nanoparticles immobilized onto poly(4â€vinylpyridine)â€functionalized magnetic nanoparticles: A robust magnetically recyclable catalyst for oxidantâ€free alcohol dehydrogenation. Applied Organometallic Chemistry, 2018, 32, e4061.	3.5	8

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37	Structural and electronic properties of alkyl-trifluoroborate based ionic liquids: A theoretical study. Journal of Fluorine Chemistry, 2013, 153, 96-100.	1.7	6
38	Interaction of Cun, Agn and Aun (nÂ= 1â€“4) nanoparticles with ChCl:Urea deep eutectic solvent. Journal of Molecular Graphics and Modelling, 2021, 105, 107866.	2.4	6
39	Refractive index prediction of deep eutectic solvents by molecular approaches. Journal of Molecular Liquids, 2021, 332, 115843.	4.9	6
40	Computational investigation of thermochemical properties of non-natural C-nucloebases: different hydrogen-bonding preferences for non-natural Watsonâ€“Crick base pairs. Structural Chemistry, 2013, 24, 1015-1025.	2.0	5
41	The interaction of deep eutectic solvents with pristine carbon nanotubes and their associated defects: A density functional theory study. Journal of Molecular Liquids, 2022, 363, 119855.	4.9	5
42	What roles do boron substitutions play in structural, tautomeric, base pairing and electronic properties of uracil? NBO & AIM analysis. Journal of Physical Organic Chemistry, 2012, 25, 787-796.	1.9	4
43	Structural and electronic properties of adsorbed nucleobases on Si-doped hexagonal boron nitride nanoflake: a computational study. Structural Chemistry, 2019, 30, 1277-1287.	2.0	4
44	DFT study of interaction of Palladium Pdn (n = 1â€“6) nanoparticles with deep eutectic solvents. Journal of Molecular Graphics and Modelling, 2022, 110, 108072.	2.4	3
45	INFLUENCE OF CATION-HETEROATOM (Li+, Na+, AND K+) INTERACTION ON THE STRUCTURAL AND THERMOCHEMICAL PROPERTIES OF 2â€²-DEOXYTHYMIDINE NUCLEOSIDE: QTAIM AND NBO ANALYZES. Journal of Theoretical and Computational Chemistry, 2013, 12, 1250113.	1.8	2
46	Effect of mono-vacant defects on the adsorption properties of deep eutectic solvents onto hexagonal boron-nitride nanoflakes. Journal of Molecular Liquids, 2022, 349, 118122.	4.9	2
47	Chemical structure-based models for prediction of density of ammonium and phosphonium-based deep eutectic solvents. Journal of Molecular Liquids, 2021, 343, 117595.	4.9	1