Sepideh Ketabi

List of Publications by Year
in descending order

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28 papers	290 citations	1039406 9 h-index	940134 16 g-index
28 all docs	28 docs citations	28 times ranked	315 citing authors

#	Article	IF	Citations
1	Carbon nanotube as a carrier in drug delivery system for carnosine dipeptide: A computer simulation study. Materials Science and Engineering C, 2017, 73, 173-181.	3.8	47
2	Encapsulation of cisplatin as an anti-cancer drug into boron-nitride and carbon nanotubes: Molecular simulation and free energy calculation. Materials Science and Engineering C, 2016, 67, 98-103.	3.8	25
3	Hydrogen adsorption capacity of vanadium oxide nanotube from pure and mixture gas environment through molecular simulation. Separation Science and Technology, 2018, 53, 1-12.	1.3	25
4	Simulation of DNA bases in water: Comparison of the Monte Carlo algorithm with molecular mechanics force fields. Biochemistry (Moscow), 2006, 71, S1-S8.	0.7	24
5	The solvation study of carbon, silicon and their mixed nanotubes in water solution. Journal of Molecular Modeling, 2012, 18, 3379-3388.	0.8	18
6	Study of DNA base-Li doped SiC nanotubes in aqueous solutions: a computer simulation study. Journal of Molecular Modeling, 2013, 19, 1605-1615.	0.8	18
7	Monte Carlo simulation study of melittin: Protein folding and temperature dependence. Russian Journal of Physical Chemistry A, 2006, 80, S55-S62.	0.1	17
8	Insight into the solvent effect on the structure, IR-spectrum, and hyperpolarizability of CpMe2Ta(benzyne), a mononuclear Tantalumâ€“benzyne complex. Russian Journal of Inorganic Chemistry, 2017, 62, 1371-1378.	0.3	15
9	Density Functional Study of Hydrogen Adsorption on Alkali Metal Doped Carbon Nanotube. Journal of Computational and Theoretical Nanoscience, 2014, 11, 1317-1322.	0.4	13
10	Complexation behaviour ofp-t-butyl-calix[4]arene propoxy derivatives toward alkali metal cations in chloroform. Physics and Chemistry of Liquids, 2006, 44, 449-456.	0.4	10
11	Complexes of pyrimidine DNA bases with thallium(I). Russian Journal of Inorganic Chemistry, 2006, 51, 1009-1013.	0.3	9
12	Solvation of alanine and histidine functionalized carbon nanotubes in aqueous media: A Monte Carlo simulation study. Journal of Molecular Liquids, 2015, 208, 191-195.	2.3	8
13	A Theoretical Study of Metal-Stabilised Rare Tautomers Stability: N4 Metalated Cytosine (M=Be2+,) Tj ETQq1 1 0.784314 rgBT /Overlock 2004, 11-18.	0.6	7
14	Hydrogen storage comparison of M doped vanadium oxide nanotubes (MÂ=ÂMo, Zr and W): A molecular simulation study. International Journal of Hydrogen Energy, 2018, 43, 2831-2839.	3.8	7
15	Molecular Simulation Study of Gold Clusters for Transporting of Thioguanine Anticancer Drug in Aqueous Solution. Journal of Cluster Science, 2022, 33, 135-143.	1.7	6
16	Complexes of Adenine and Guanine with Thallium(I). Main Group Metal Chemistry, 2004, 27, .	0.6	5
17	Theoretical Study of the Interactions between Isolated DNA Bases and Various Groups IA and IIA Metal Ions by Ab Initio Calculations. Monatshefte FÃ¼r Chemie, 2008, 139, 89-100.	0.9	5
18	Potentiality of carbon nanotube to encapsulate some alkylating agent anticancer drugs: a molecular simulation study. Structural Chemistry, 2021, 32, 869-877.	1.0	5

#	Article	IF	Citations
19	DFT based QSAR study on quinolone-triazole derivatives as antibacterial agents. Journal of Receptor and Signal Transduction Research, 2021, , 1-11.	1.3	5
20	QSAR study of antituberculosis activity of oxadiazole derivatives using DFT calculations. Journal of Receptor and Signal Transduction Research, 2022, , 1-9.	1.3	5
21	Solvation free energies of glutamate and its metal complexes: A computer simulation study. Journal of Molecular Modeling, 2011, 17, 889-898.	0.8	4
22	Computer Simulation Study of the Interactions Between Gold Clusters and Glutamate in Aqueous Solution. Journal of Solution Chemistry, 2015, 44, 2027-2041.	0.6	3
23	A Computational Understanding of Solvent Effect on the Structure, Electronic, Thermochemical, and Spectroscopic Properties of Ni(I-2-C6H4)(H2PCH2CH2PH2) Complex. Journal of the Chinese Chemical Society, 2017, 64, 925-933.	0.8	3
24	Quantum simulation on donor and acceptor II calix[4]arene substrate and alkali metal ions: the driven inclusion. Physics and Chemistry of Liquids, 2007, 45, 425-433.	0.4	2
25	The competitive interactions between the anion-receptor, anions and neutral solvent species. Journal of Power Sources, 2009, 194, 58-65.	4.0	2
26	Effect of metal doping on the solvation of carbon nanotubes: a Monte Carlo simulation study. Physics and Chemistry of Liquids, 2014, 52, 763-776.	0.4	1
27	CO2 & CH4 Capture and Separation Using Ti Doped Vanadium Oxide Nanotube: Molecular Simulation Study. Separation Science and Technology, 0, , 1-16.	1.3	1
28	Simulation Study of Li Doped Carbon Nanotube as A Carrier System for Aspirin in Aqueous Media. Nano Biomedicine and Engineering, 2015, 7, .	0.3	0