Heidar Raissi

List of Publications by Year
in descending order

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91	2,330	172457	254184
papers	citations	29	43
		h-index	g-index

91	91	91	1413
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Understanding loading, diffusion and releasing of Doxorubicin and Paclitaxel dual delivery in graphene and graphene oxide carriers as highly efficient drug delivery systems. Applied Surface Science, 2020, 500, 144220.	6.1	88
2	Assessment of the adsorption mechanism of Flutamide anticancer drug on the functionalized single-walled carbon nanotube surface as a drug delivery vehicle: An alternative theoretical approach based on DFT and MD. Applied Surface Science, 2018, 434, 492-503.	6.1	87
3	DFT Calculations and Molecular Dynamics Simulation Study on the Adsorption of 5-Fluorouracil Anticancer Drug on Graphene Oxide Nanosheet as a Drug Delivery Vehicle. Journal of Inorganic and Organometallic Polymers and Materials, 2017, 27, 805-817.	3.7	80
4	The hybrid of Pd and SWCNT (Pd loaded on SWCNT) as an efficient sensor for the formaldehyde molecule detection: A DFT study. Sensors and Actuators B: Chemical, 2015, 212, 55-62.	7.8	75
5	Covalent organic framework as smart and high efficient carrier for anticancer drug delivery: a DFT calculations and molecular dynamics simulation study. Journal Physics D: Applied Physics, 2018, 51, 345401.	2.8	73
6	On the pseudocapacitive behavior of nanostructured molybdenum oxide. Journal of Solid State Electrochemistry, 2010, 14, 643-650.	2.5	60
7	Theoretical study of solvent and co-solvent effects on the interaction of Flutamide anticancer drug with Carbon nanotube as a drug delivery system. Journal of Molecular Liquids, 2017, 248, 490-500.	4.9	60
8	Screening of the structural, topological, and electronic properties of the functionalized Graphene nanosheets as potential Tegafur anticancer drug carriers using DFT method. Journal of Biomolecular Structure and Dynamics, 2018, 36, 2517-2529.	3.5	60
9	Density functional theory calculations and molecular dynamics simulations of the adsorption of ellipticine anticancer drug on graphene oxide surface in aqueous medium as well as under controlled pH conditions. Journal of Molecular Liquids, 2018, 255, 269-278.	4.9	56
10	Solvent/co-solvent effects on the electronic properties and adsorption mechanism of anticancer drug Thioguanine on Graphene oxide surface as a nanocarrier: Density functional theory investigation and a molecular dynamics. Applied Surface Science, 2017, 422, 1030-1041.	6.1	55
11	Solvent effects on the stability and the electronic properties of histidine/Pd-doped single-walled carbon nanotube biosensor. Journal of Molecular Liquids, 2016, 214, 313-318.	4.9	53
12	Investigation of the solvent effect, molecular structure, electronic properties and adsorption mechanism of Tegafur anticancer drug on Graphene nanosheet surface as drug delivery system by molecular dynamics simulation and density functional approach. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2017, 88, 159-169.	1.6	53
13	Assessment of solvent effects on the interaction of Carmustine drug with the pristine and COOH-functionalized single-walled carbon nanotubes: A DFT perspective. Journal of Molecular Liquids, 2017, 240, 87-97.	4.9	52
14	The functionalization of carbon nanotubes to enhance the efficacy of the anticancer drug paclitaxel: a molecular dynamics simulation study. Journal of Molecular Modeling, 2017, 23, 222.	1.8	52
15	DFT and MD investigations on the functionalized boron nitride nanotube as an effective drug delivery carrier for Carmustine anticancer drug. Journal of Molecular Liquids, 2019, 276, 577-587.	4.9	49
16	Immunosuppressive agent leflunomide: A SWNTs-immobilized dihydroortate dehydrogenase inhibitory effect and computational study of its adsorption properties on zigzag single walled (6,0) carbon and boron nitride nanotubes as controlled drug delivery devices. European Journal of Pharmaceutical Sciences, 2014, 56, 37-54.	4.0	46
17	Assessment of adsorption behavior of 5-fluorouracil and pyrazinamide on carbon nitride and folic acid-conjugated carbon nitride nanosheets for targeting drug delivery. Journal of Molecular Liquids, 2020, 301, 112435.	4.9	42
18	Substituent effect on structure, electron density, and intramolecular hydrogen bonding in nitrosoâ€oxime methane. International Journal of Quantum Chemistry, 2011, 111, 3505-3516.	2.0	41

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19	The effects of substitutions on structure, electron density, resonance and intramolecular hydrogen bonding strength in 3-mercapto-propenethial. Computational and Theoretical Chemistry, 2010, 960, 1-9.	1.5	40
20	Investigation of graphene-based nanomaterial as nanocarrier for adsorption of paclitaxel anticancer drug: a molecular dynamics simulation study. Journal of Molecular Modeling, 2017, 23, 36.	1.8	40
21	Strong intramolecular hydrogen bond in triformylmethane ab-initio, AIM and NBO study. Computational and Theoretical Chemistry, 2006, 759, 93-100.	1.5	38
22	Ab initio and DFT computational studies on molecular conformations and strength of the intramolecular hydrogen bond in different conformers of 3-amino-2-iminomethyl acryl aldehyde. Computational and Theoretical Chemistry, 2011, 966, 299-305.	2.5	38
23	Comprehensive study of the interaction between hydrogen halides and methanol derivatives. International Journal of Quantum Chemistry, 2012, 112, 2782-2786.	2.0	37
24	The analysis of electronic structures, adsorption properties, NBO, QTAIM and NMR parameters of the adsorbed hydrogen sulfide on various sites of the outer surface of aluminum phosphide nanotube: a DFT study. Structural Chemistry, 2015, 26, 1059-1075.	2.0	37
25	Molecular dynamics simulation and quantum chemical studies on the investigation of aluminum nitride nanotube as phosgene gas sensor. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 86, 305-322.	1.6	37
26	Understanding co-loading of doxorubicin and camptothecin on graphene and folic acid-conjugated graphene for targeting drug delivery: classical MD simulation and DFT calculation. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2737-2745.	3.5	36
27	Conformational study of the (z)-[(2-iminoethylidone)silyl]amine at the MP2, DFT and G2MP2 levels. Computational and Theoretical Chemistry, 2012, 983, 1-6.	2.5	35
28	Investigation of the molecular structure, electronic properties, AIM, NBO, NMR and NQR parameters for the interaction of Sc, Ga and Mg-doped (6,0) aluminum nitride nanotubes with COCl2 gas by DFT study. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 84, 99-114.	1.6	34
29	Assessment of the chitosan-functionalized graphene oxide as a carrier for loading thioguanine, an antitumor drug and effect of urea on adsorption process: Combination of DFT computational and molecular dynamics simulation studies. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2487-2497.	3.5	31
30	Payload delivery of anticancer drug Tegafur with the assistance of graphene oxide nanosheet during biomembrane penetration: Molecular dynamics simulation survey. Applied Surface Science, 2020, 517, 146186.	6.1	29
31	Assessment of solvent effects on the inclusion behavior of pyrazinamide drug into cyclic peptide based nanotubes as novel drug delivery vehicles. Journal of Molecular Liquids, 2018, 268, 326-334.	4.9	28
32	The computational study of the Î³-Fe₂O₃ nanoparticle as Carmustine drug delivery system: DFT approach. Journal of Biomolecular Structure and Dynamics, 2019, 37, 454-464.	3.5	28
33	Loading and release of anticancer drug from phosphorene as a template material with high efficient carrier: From vacuum to cell membrane. Journal of Molecular Liquids, 2019, 291, 111346.	4.9	26
34	Comparative prediction of binding affinity of Hydroxyurea anti-cancer to boron nitride and carbon nanotubes as smart targeted drug delivery vehicles. Journal of Biomolecular Structure and Dynamics, 2019, 37, 4852-4862.	3.5	26
35	Probing the adsorption and release mechanisms of cytarabine anticancer drug on/from dopamine functionalized graphene oxide as a highly efficient drug delivery system. Journal of Molecular Liquids, 2020, 301, 112458.	4.9	26
36	Electronic structures, intramolecular hydrogen bond interaction, and aromaticity of substituted 4-amino-3-penten-2-one in ground and electronic excited state. Structural Chemistry, 2015, 26, 491-506.	2.0	25

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37	Investigation of the Pristine and Functionalized Carbon Nanotubes as a Delivery System for the Anticancer Drug Dacarbazine: Drug Encapsulation. Journal of Pharmaceutical Sciences, 2021, 110, 2005-2016.	3.3	25
38	Using molecular dynamics simulation to explore the binding of the three potent anticancer drugs sorafenib, streptozotocin, and sunitinib to functionalized carbon nanotubes. Journal of Molecular Modeling, 2019, 25, 159.	1.8	24
39	Stabilization of d-lactate dehydrogenase diagnostic enzyme via immobilization on pristine and carboxyl-functionalized carbon nanotubes, a combined experimental and molecular dynamics simulation study. Archives of Biochemistry and Biophysics, 2019, 661, 178-186.	3.0	24
40	The influence of nicotine on pioglitazone encapsulation into carbon nanotube: the investigation of molecular dynamic and density functional theory. Journal of Biomolecular Structure and Dynamics, 2017, 35, 520-534.	3.5	23
41	A combined molecular dynamics simulation and quantum mechanics study on mercaptopurine interaction with the cucurbit [6,7] urils: Analysis of electronic structure. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 188, 647-658.	3.9	23
42	Interactions of the 5-fluorouracil anticancer drug with DNA pyrimidine bases: a detailed computational approach. Structural Chemistry, 2016, 27, 487-504.	2.0	22
43	Theoretical elucidation of the amino acid interaction with graphene and functionalized graphene nanosheets: insights from DFT calculation and MD simulation. Amino Acids, 2020, 52, 1465-1478.	2.7	22
44	Comprehensive theoretical prediction of the dynamics and stability properties of Tegafur pharmaceutical agent on the Graphene based nanostructures in aqueous environment. Applied Surface Science, 2018, 455, 32-36.	6.1	21
45	Modeling the interaction between anti-cancer drug penicillamine and pristine and functionalized carbon nanotubes for medical applications: density functional theory investigation and a molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1322-1334.	3.5	20
46	DFT and MD study of adsorption sensitivity of aluminium phosphide nanotube towards some air pollutant gas molecules. Molecular Simulation, 2017, 43, 675-690.	2.0	19
47	Understanding the effect of vitamin B6 and PEG functionalization on improving the performance of carbon nanotubes in temozolomide anticancer drug transportation. Journal Physics D: Applied Physics, 2019, 52, 395402.	2.8	19
48	Design of a new drug delivery platform based on surface functionalization 2D covalent organic frameworks. Journal of the Taiwan Institute of Chemical Engineers, 2021, 125, 15-22.	5.3	19
49	Ab initioand DFT computational studies on molecular conformations and intramolecular hydrogen bonding in 3-mercapto-but-2-enethial. Journal of Sulfur Chemistry, 2010, 31, 275-285.	2.0	18
50	Theoretical study of the effects of substitution, solvation, and structure on the interaction between nitriles and methanol. International Journal of Quantum Chemistry, 2012, 112, 1273-1284.	2.0	17
51	Carbon and boron nanotubes as a template material for adsorption of 6-Thioguanine chemotherapeutic: a molecular dynamics and density functional approach. Journal of Biomolecular Structure and Dynamics, 2020, 38, 697-707.	3.5	17
52	Investigation of nanotubes as the smart carriers for targeted delivery of mercaptopurine anticancer drug. Journal of Biomolecular Structure and Dynamics, 2022, 40, 4579-4592.	3.5	16
53	Enhance the efficiency of 5-fluorouracil targeted delivery by using a prodrug approach as a novel strategy for prolonged circulation time and improved permeation. International Journal of Pharmaceutics, 2019, 568, 118491.	5.2	15
54	DFT computational study towards investigating Cladribine anticancer drug adsorption on the graphene and functionalized graphene. Structural Chemistry, 2020, 31, 1691-1705.	2.0	15

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55	A density functional theory-based analysis of the structural, topological and electronic properties of gemcitabine drug adsorption on the pyrrolidine functionalized single-walled carbon nanotube. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2477-2486.	3.5	14
56	Solvent effects on the structural, electronic properties and intramolecular Nâ€“H O hydrogen bond strength of 5-aminomethylene-pyrimidine-2,4,6 trion with DFT calculations. Journal of Molecular Liquids, 2016, 215, 77-87.	4.9	13
57	Adsorption of Ampyra anticancer drug on the graphene and functionalized graphene as template materials with high efficient carrier. Adsorption, 2020, 26, 879-893.	3.0	13
58	Effect of substitution on the intramolecular hydrogen bonding of 4-amino-3-penten-2-one: Ab initio, AIM and NBO studies. Computational and Theoretical Chemistry, 2007, 847, 47-51.	1.5	12
59	Density functional theory study towards investigating the adsorption properties of the Î³-Fe2O3 nanoparticles as a nanocarrier for delivery of Flutamide anticancer drug. Adsorption, 2020, 26, 925-939.	3.0	12
60	Evaluation of solvent and ion effects upon leflunomide adsorption characteristics on (6,0) zigzag single-walled carbon nanotube and immobilized dihydroorotate dehydrogenase activity: A computational DFT and experimental study. Journal of Molecular Liquids, 2017, 231, 528-541.	4.9	11
61	Analysis of the structures, energetics, and vibrational frequencies for the hydrogen-bonded interaction of nucleic acid bases with Carmustine pharmaceutical agent: a detailed computational approach. Structural Chemistry, 2018, 29, 1165-1174.	2.0	11
62	Molecular insights into the loading and dynamics of anticancer drugs on silicene and folic acid-conjugated silicene nanosheets: DFT calculation and MD simulation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 3892-3899.	3.5	11
63	Investigation of adsorption properties of CS2 on interior and exterior surfaces of single-walled silicon-carbide nanotubes and effect of applied electric field: electronic structure, charge density and NMR studies. RSC Advances, 2015, 5, 84022-84037.	3.6	10
64	Theoretical Prediction of Adsorption Properties of Carmustine Drug on Various Sites of the Outer Surface of the Single-Walled Boron Nitride Nanotube and Investigation of Urea Effect on Drug Delivery by DFT and MD. Journal of Cluster Science, 2018, 29, 93-99.	3.3	10
65	Conjugation of a smart polymer to doxorubicin through a pH-responsive bond for targeted drug delivery and improving drug loading on graphene oxide. RSC Advances, 2021, 11, 18809-18817.	3.6	10
66	Doped-SiCNT as a promising sensor for detection of CS₂ molecule. Journal of Sulfur Chemistry, 2017, 38, 372-383.	2.0	9
67	Assessment of dynamical properties of mercaptopurine on the peptide-based metalâ€“organic framework in response to experience of external electrical fields: a molecular dynamics simulation. Journal of Molecular Modeling, 2019, 25, 304.	1.8	9
68	Molecular mechanism for the encapsulation of the doxorubicin in the cucurbit[n]urils cavity and the effects of diameter, protonation on loading and releasing of the anticancer drug:Mixed quantum mechanical/ molecular dynamics simulations. Computer Methods and Programs in Biomedicine, 2020, 196, 105563.	4.7	9
69	Design of new drug delivery platform based on surface functionalization of black phosphorus nanosheet with a smart polymer for enhancing the efficiency of doxorubicin in the treatment of cancer. Journal of Biomedical Materials Research - Part A, 2021, 109, 1912-1921.	4.0	9
70	The performance of the single-walled carbon nanotube covalently modified with polyethylene glycol to delivery of Gemcitabine anticancer drug in the aqueous environment. Journal of Biomolecular Structure and Dynamics, 2021, 39, 881-888.	3.5	9
71	Effects of the HCN adsorption on the structural and electronic parameters of the beryllium oxide nanotube. Structural Chemistry, 2016, 27, 557-571.	2.0	8
72	Theoretical investigation insights into the temperature triggered tegafur anticancer drug release from the surface of graphene oxide nanosheet. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2287-2295.	3.5	8

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73	Two dimensional porous frameworks of graphyne family as therapeutic delivery vehicles for Idarubicin biomolecule in silico: Density functional theory and molecular dynamics simulation. Journal of Molecular Liquids, 2020, 319, 114334.	4.9	8
74	Understanding dual delivery of doxorubicin and paclitaxel with boron nitride and phosphorene nanosheets as highly efficient drug delivery systems. Journal of Biomolecular Structure and Dynamics, 2021, 39, 5613-5618.	3.5	8
75	Development and evaluation of a pH-responsive and water-soluble drug delivery system based on smart polymer coating of graphene nanosheets: an in silico study. RSC Advances, 2020, 10, 31106-31114.	3.6	8
76	New insights into Hexakis macrocycles as a novel nano-carrier for highly potent anti-cancer treatment: A new challenge in drug delivery. Colloids and Surfaces B: Biointerfaces, 2021, 197, 111402.	5.0	8
77	Molecular interpretation of the carbon nitride performance as a template for the transport of anti-cancer drug into the biological membrane. Scientific Reports, 2021, 11, 18981.	3.3	8
78	CONFORMATIONAL PROPERTIES AND INTRAMOLECULAR HYDROGEN BONDING OF 3-AMINO-PROPENESELENAL: AN AB INITIO AND DENSITY FUNCTIONAL THEORY STUDIES. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350025.	1.8	7
79	Theoretical calculations of intramolecular hydrogen bond of the 2-Amino-2, 4, 6-cycloheptatrien-1-one in the gas phase and solution: Substituent effects and their positions. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650063.	1.8	7
80	Predicting the efficiency of polyethylene glycol-functionalised graphene in delivery of temozolomide anticancer drug and investigating the effect of pH on the drug release process: DFT and free energy calculations. Molecular Simulation, 2020, 46, 1474-1482.	2.0	7
81	The transport of Idarubicin therapeutic agent using a novel graphene sheet as a drug delivery platform through a biomembrane. Journal of Molecular Liquids, 2021, 323, 115050.	4.9	7
82	Molecular dynamics simulation study of Glycine tip-functionalisation of single-walled carbon nanotubes as emerging nanovectors for the delivery of anticancer drugs. Molecular Simulation, 2020, 46, 111-120.	2.0	6
83	Assessment of the effect of external and internal triggers on adsorption and release of paclitaxel from the PEI functionalized silicene nanosheet: A molecular dynamic simulation. Journal of Molecular Graphics and Modelling, 2021, 106, 107930.	2.4	6
84	Molecular insight into the role of polyethylene glycol and cholesterol on the performance of graphene-based nanomaterials in Blood-brain barrier delivery. Journal of Molecular Liquids, 2021, 341, 117446.	4.9	6
85	Cation-pi interaction: A strategy for enhancing the performance of graphene-based drug delivery systems. Inorganic Chemistry Communication, 2022, 141, 109542.	3.9	6
86	The effects of electrolyte on the capacitive behavior of nanostructured molybdenum oxides. Journal of Chemical Technology and Biotechnology, 2019, 94, 3800-3805.	3.2	5
87	Conformational and tautomeric preferences in 3â€aminoacrylaldehyde: A theoretical study. International Journal of Quantum Chemistry, 2011, 111, 586-595.	2.0	4
88	Boosting BeONT Reactivity with HCN by Calcium and Magnesium Doping: A DFT Investigation of Electronic Structure, AIM, NMR, NQR and NBO Analysis. Journal of Cluster Science, 2018, 29, 101-110.	3.3	4
89	A new insight into the transfer and delivery of anti-SARS-CoV-2 drug Carmofur with the assistance of graphene oxide quantum dot as a highly efficient nanovector toward COVID-19 by molecular dynamics simulation. RSC Advances, 2022, 12, 14167-14174.	3.6	4
90	In silico exploration of disulfide derivatives of Ferula foetida oleo-gum (CovexirÂ®) as promising therapeutics against SARS-CoV-2. Computers in Biology and Medicine, 2022, , 105566.	7.0	1

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91	Understanding the role of hydrogen bonds in destruction of DNA by screening interactions of Flutamide anticancer drug with nucleotides bases: DFT perspective, MD simulation and free energy calculation. Adsorption, 2020, 26, 491-508.	3.0	0