Mehrnoosh Khaleghian

List of Publications by Year
in descending order

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21	296	933447 10	888059 17
papers	citations	h-index	g-index

22	22	22	177
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Interaction Between New Anti-cancer Drug Syndros and CNT(6,6-6) Nanotube for Medical Applications: Geometry Optimization, Molecular Structure, Spectroscopic (NMR, UV/Vis, Excited state), FMO, MEP and HOMO-LUMO Investigation. Applied Surface Science, 2018, 434, 504-513.	6.1	57
2	Adsorption properties of the molecule resveratrol on CNT(8,0-10) nanotube: Geometry optimization, molecular structure, spectroscopic (NMR, UV/Vis, excited state), FMO, MEP and HOMO-LUMO investigations. Journal of Molecular Structure, 2018, 1160, 479-487.	3.6	54
3	New derivatives of (E,E)-azomethines: Design, quantum chemical modeling, spectroscopic (FT-IR, UV/Vis,) Tj ETQq1 1 0.784314 rgBT /Ov Journal of Molecular Structure, 2018, 1152, 368-385.	3.6	28
4	Synthesis, geometry optimization, spectroscopic investigations (UV/Vis, excited states, FT-IR) and application of new azomethine dyes. Journal of Molecular Structure, 2017, 1148, 134-149.	3.6	26
5	Interaction between new synthesized derivative of (E,E)-azomethines and BN(6,6-7) nanotube for medical applications: Geometry optimization, molecular structure, spectroscopic (NMR, UV/Vis,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 881-888.	3.6	19
6	Design of geometry, synthesis, spectroscopic (FT-IR, UV/Vis, excited state, polarization) and anisotropy (thermal conductivity and electrical) properties of new synthesized derivatives of (E,E)-azomethines in colored stretched poly (vinyl alcohol) matrix. Journal of Molecular Structure, 2018, 1157, 536-550.	3.6	18
7	Spectroscopic Studies (Geometry Optimization, E â†' Z Isomerization, UV/Vis, Excited States, FT-IR,) Tj ETQq1 1 0.784314 rgBT /Overlo New Azomethine Dyes in Stretched Polymer Matrix. Silicon, 2018, 10, 2361-2385.	3.3	14
8	Theoretical study of encapsulation of Floxuridine anticancer drug into BN (9,9-7) nanotube for medical application. Phosphorus, Sulfur and Silicon and the Related Elements, 2020, 195, 293-306.	1.6	13
9	DFT Study and NBO Analysis of Conformational Properties of 2-Substituted 2-Oxo-1,3,2-Dioxaphosphorinanes and Their Dithia and Diselena Analogs. Letters in Organic Chemistry, 2015, 12, 516-522.	0.5	13
10	Investigation of the Adsorption Rubraca Anticancer Drug on the CNT(4,4-8) Nanotube as a Factor of Drug Delivery: A Theoretical Study Based on DFT Method. Current Molecular Medicine, 2019, 19, 473-486.	1.3	12
11	Investigation of encapsulation of Talzenna drug into carbon and boron-nitride nanotubes [CNT(8,8-7) and BNNT(8,8-7)]: a DFT study. Chemical Papers, 2021, 75, 1521-1533.	2.2	10
12	DFT study of physisorption effect of CO and CO2 on furanocoumarins for air purification. Journal of Environmental Chemical Engineering, 2018, 6, 4784-4796.	6.7	9
13	Theoretical Investigation of Interaction 7-Hydroxy Phenothiazine 3-One Dye with Nanotube: a DFT Study. Russian Journal of Physical Chemistry B, 2021, 15, 170-182.	1.3	6
14	Characterization of the binding affinity between some anti-Parkinson agents and Mn2+, Fe3+ and Zn2+ metal ions: A DFT insight. Inorganic Chemistry Communication, 2021, 128, 108582.	3.9	5
15	Study of the Adsorption Antioxidant Compound Malva on the BNNT(9,9-9): An Investigation based on DFT Method. Russian Journal of Physical Chemistry B, 2022, 16, 175-184.	1.3	5
16	Theoretical modelling of encapsulation of the Altretamine drug into BN(9,9-5) and AlN(9,9-5) nano rings: a DFT study. Molecular Physics, 2019, 117, 2559-2569.	1.7	4
17	DFT Study of Adsorption of (4E,6E)-4-(4-Hydroxyphenyldiazenyl)-N-((furan-2-yl)methylene)benzenamine on BN(6,6-8) Nanotube. Russian Journal of Physical Chemistry A, 2020, 94, 778-788.	0.6	1
18	Evaluating role of the xâ€"Ï€ (xâ€‰=â€‰Ï€ and/or CH) stacking interactions in adsorption of the (4E,4E)-4-(4-hydroxyphenyldiazenyl)-N-((furan-2-Yl)methylene)benzenamine antibacterial in armchair boron nitride nanotube. Chemical Papers, 2020, 74, 2991-3000.	2.2	1

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19	Quantum Mechanical Investigation of Geometrical Structure and Dynamic Behavior of h-BNNT (9,9-5) and h-AlNNT (9,9-5)Single-Walled Nanotubes: NBO Analysis. Letters in Organic Chemistry, 2019, 16, 705-717.	0.5	1
20	Theoretical Study of Non-Bonded Interaction between Anticancer Drug Fludara and (2S,3R,4S,5S)-2-(Hydroxymethyl)-3,5-dimethyloxolane-3,4-diol: A DFT Study. Russian Journal of Physical Chemistry A, 2021, 95, 127-138.	0.6	0
21	Investigation of Adsorption Effect of Carbon Monoxide on Coniine: A DFT Study. Letters in Organic Chemistry, 2021, 17, .	0.5	0