

Mehrnoosh Khaleghian

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/10662648/publications.pdf>

Version: 2024-02-01

21
papers

296
citations

933447

10
h-index

888059

17
g-index

22
all docs

22
docs citations

22
times ranked

177
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	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
3	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
4	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
5	Investigation of Adsorption Effect of Carbon Monoxide on Coniine: A DFT Study. Letters in Organic Chemistry, 2021, 17, .	0.5	0
6	Characterization of the binding affinity between some anti-Parkinson agents and Mn ²⁺ , Fe ³⁺ and Zn ²⁺ metal ions: A DFT insight. Inorganic Chemistry Communication, 2021, 128, 108582.	3.9	5
7	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
8	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
9	Evaluating role of the π - π (C=C 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
10	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
11	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
12	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
13	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
14	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
15	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
16	New derivatives of (E,E)-azomethines: Design, quantum chemical modeling, spectroscopic (FT-IR, UV/Vis,) Tj ETQq0 0 0 rgBT /Overlock 1 Journal of Molecular Structure, 2018, 1152, 368-385.	3.6	28
17	Spectroscopic Studies (Geometry Optimization, E \rightarrow Z Isomerization, UV/Vis, Excited States, FT-IR,) Tj ETQq1 1 0.784314 rgBT /Overlock New Azomethine Dyes in Stretched Polymer Matrix. Silicon, 2018, 10, 2361-2385.	3.3	14
18	DFT study of physisorption effect of CO and CO ₂ on furanocoumarins for air purification. Journal of Environmental Chemical Engineering, 2018, 6, 4784-4796.	6.7	9

#	ARTICLE	IF	CITATIONS
19	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 0.7843314 rgBT /Oyerlock 10 881-888.	3.6	19
20	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
21	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