S Vijayakumar

List of Publications by Year
in descending order

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26	355	933447 10	839539 18
papers	citations	h-index	g-index

26	26	26	434
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Amine terminated polyynes as candidates for molecular wire applications: A DFT study. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 137, 115045.	2.7	3
2	Highly delocalised molecular orbitals in boron-, carbon- and nitrogen-based linear chains: a DFT study. Molecular Physics, 2022, 120, .	1.7	3
3	Adsorption of volatile organic compounds on pristine and defected nanographene. Computational and Theoretical Chemistry, 2022, 1211, 113664.	2.5	9
4	Adsorption of greenhouse gases on the surface of covalent organic framework of porphyrin â€“ An ab initio study. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 126, 114448.	2.7	8
5	Functionalized oligoynes: comparison of theoretical parameters with experimental single molecule conductance. Structural Chemistry, 2021, 32, 1795-1806.	2.0	4
6	Polyyne-metal complexes for use in molecular wire applications: A DFT insight. Computational and Theoretical Chemistry, 2021, 1202, 113328.	2.5	3
7	Structural insights into the anti-cancer activity of quercetin on G-tetrad, mixed G-tetrad, and G-quadruplex DNA using quantum chemical and molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2020, 38, 317-339.	3.5	31
8	DFT approach on stability and conductance of nine different polyyne and cumulene molecules. Molecular Physics, 2020, 118, .	1.7	5
9	Ab initio studies of adsorption of Haloarenes on Heme group. Journal of Molecular Modeling, 2020, 26, 6.	1.8	6
10	Structural exploration of viral matrix protein 40 interaction with the transition metal ions (Ag⁺ and Cu²⁺). Journal of Biomolecular Structure and Dynamics, 2019, 37, 2875-2896.	3.5	8
11	Modeling of 2-D hydrogen-edge capped defected & boron-doped defected graphene sheets for the adsorption of CO2, SO2 towards energy harvesting applications. Applied Surface Science, 2019, 463, 596-609.	6.1	34
12	Theoretical insights into the metal chelating and antimicrobial properties of the chalcone based Schiff bases. Molecular Simulation, 2019, 45, 636-645.	2.0	19
13	Mechanistic insights into the inhibition mechanism of cysteine cathepsins by chalcone-based inhibitorsâ€"a QM cluster model approach. Structural Chemistry, 2019, 30, 1779-1793.	2.0	2
14	Density functional theory study on the adsorption of alkali metal ions with pristine and defected graphene sheet. Molecular Physics, 2019, 117, 462-473.	1.7	22
15	Role of 6-Mercaptopurine in the potential therapeutic targets DNA base pairs and G-quadruplex DNA: insights from quantum chemical and molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2018, 36, 1369-1401.	3.5	16
16	Metal chelating ability and antioxidant properties of Curcumin-metal complexes â€“ A DFT approach. Journal of Molecular Graphics and Modelling, 2018, 79, 1-14.	2.4	81
17	Reduced bond length alternation and helical molecular orbitals in donor and acceptor substituted linear carbon chains. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850049.	1.8	9
18	Effect of side chain edge functionalization in pristine and defected graphene-DFT study. Computational and Theoretical Chemistry, 2018, 1135, 34-47.	2.5	6

#	Article	IF	Citations
19	A theoretical study on the reaction mechanism and kinetics of allyl alcohol (CH₂ =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 895-911.	1.7	16
20	Adsorption of Mn atom on pristine and defected graphene: a density functional theory study. Journal of Molecular Modeling, 2017, 23, 132.	1.8	12
21	DFT-based investigation on adsorption of methane on pristine and defected graphene. Structural Chemistry, 2017, 28, 1935-1952.	2.0	35
22	Interaction studies of human prion protein (HuPrP109â€“111: methionine-lysine-histidine) tripeptide model with transition metal cations. Journal of Molecular Graphics and Modelling, 2016, 69, 111-126.	2.4	2
23	Mechanism and kinetics of the atmospheric degradation of 2-formylcinnamaldehyde with O₃ and hydroxyl OH radicals â€“ a theoretical study. Molecular Physics, 2016, 114, 3055-3075.	1.7	11
24	Reaction mechanism of HSH and CH₃SH with NH₂CH₂COCH₂X (X = F and Cl) molecules. International Journal of Quantum Chemistry, 2008, 108, 927-936.	2.0	5
25	Isomerization study of C5H5NO molecules. International Journal of Quantum Chemistry, 2007, 107, 769-781.	2.0	1
26	Isomerization of C3H3NO isomers:ab initiostudy. Molecular Physics, 2006, 104, 1401-1411.	1.7	4