Amirali Abbasi

List of Publications by Year
in descending order

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39 papers	1,142 citations	394421 19 h-index	377865 34 g-index
39 all docs	39 docs citations	39 times ranked	670 citing authors

#	Article	IF	Citations
1	In silico studies of the interaction of the colon cancer receptor and RNA aptamer adsorbed on (1 0 1) facet of TiO2 nanoparticle investigated by molecular dynamics simulation. Adsorption, 2020, 26, 941-954.	3.0	5
2	A DFT study on the possibility of embedding a single Ti atom into the perfect stanene monolayer as a highly efficient gas sensor. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	10
3	The adsorption of sulfur trioxide and ozone molecules on stanene nanosheets investigated by DFT: Applications to gas sensor devices. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 108, 382-390.	2.7	66
4	Band gap tunability and structural stability of metal/nonmetal codoped group-IV tin nanotubes: Effect of spin-orbit coupling. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 114, 113644.	2.7	13
5	Adsorption of CO and NO molecules on Al, P and Si embedded MoS2 nanosheets investigated by DFT calculations. Adsorption, 2019, 25, 1001-1017.	3.0	33
6	Tuning the structural and electronic properties and chemical activities of stanene monolayers by embedding 4d Pd: a DFT study. RSC Advances, 2019, 9, 16069-16082.	3.6	40
7	Theoretical Investigation of The interaction Between Noble Metals (Ag, Au, Pd, Pt) and Stanene Nanosheets: A DFT Study. Journal of Inorganic and Organometallic Polymers and Materials, 2019, 29, 1895-1915.	3.7	20
8	Investigation of TiO2 anatase (1 0 1), (1 0 0) and (1 1 0) facets as immobilizer for a potential anticancer RNA aptamer: a classical molecular dynamics simulation. Molecular Simulation, 2019, 45, 849-858.	2.0	10
9	Modulation of the electronic properties of pristine and AlP-codoped stanene monolayers by the adsorption of CH₂O and CH₄ molecules: a DFT study. Materials Research Express, 2019, 6, 076410.	1.6	21
10	DFT study of the effects of Al P pair doping on the structural and electronic properties of stanene nanosheets. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 108, 34-43.	2.7	46
11	Adsorption of O3, SO2 and SO3 gas molecules on MoS2 monolayers: A computational investigation. Applied Surface Science, 2019, 469, 781-791.	6.1	150
12	TiO2-Based Nanocarriers for Drug Delivery. , 2019, , 205-248.		5
13	Adsorption of phenol, hydrazine and thiophene on stanene monolayers: A computational investigation. Synthetic Metals, 2019, 247, 26-36.	3.9	52
14	TiO2/GRAPHENE OXIDE HETEROSTRUCTURES FOR GAS-SENSING: INTERACTION OF NITROGEN DIOXIDE WITH THE PRISTINE AND NITROGEN MODIFIED NANOSTRUCTURES INVESTIGATED BY DFT. Surface Review and Letters, 2019, 26, 1850170.	1.1	4
15	Exploration of sensing of nitrogen dioxide and ozone molecules using novel TiO2/Stanene heterostructures employing DFT calculations. Applied Surface Science, 2018, 442, 368-381.	6.1	49
16	Density functional theory investigation of the interactions between the buckled stanene nanosheet and XO2 gases (Xâ€¯=â€¯N, S, C). Computational and Theoretical Chemistry, 2018, 1125, 15-28.	2.5	27
17	Structural and electronic properties of nitrogen-doped TiO2 nanocrystals and their effects on the adsorption of CH2O and SO2 molecules investigated by DFT. Journal of the Iranian Chemical Society, 2018, 15, 1431-1448.	2.2	4
18	An Innovative Method for the Removal of Toxic SOx Molecules from Environment by TiO2/Stanene Nanocomposites: A First-Principles Study. Journal of Inorganic and Organometallic Polymers and Materials, 2018, 28, 1901-1913.	3.7	8

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19	ADSORPTION OF THIOPHENE ON N-DOPED TiO₂/MoS₂ NANOCOMPOSITES INVESTIGATED BY VAN DER WAALS CORRECTED DENSITY FUNCTIONAL THEORY. Surface Review and Letters, 2018, 25, 1850038.	1.1	2
20	Theoretical study of the structural and electronic properties of novel stanene-based buckled nanotubes and their adsorption behaviors. Applied Surface Science, 2018, 435, 733-742.	6.1	22
21	Investigation of the adsorption of ozone molecules on TiO2/WSe2 nanocomposites by DFT computations: Applications to gas sensor devices. Applied Surface Science, 2018, 436, 27-41.	6.1	90
22	A highly sensitive chemical gas detecting device based on N-doped ZnO as a modified nanostructure media: A DFT+NBO analysis. Surface Science, 2018, 668, 150-163.	1.9	15
23	Structural and electronic properties of group-IV tin nanotubes and their effects on the adsorption of SO2 molecules: Insights from DFT computations. Journal of Applied Physics, 2018, 124, .	2.5	42
24	Interaction of sulfur trioxide molecules with armchair and zigzag stanene-based nanotubes: electronic properties exploration by DFT calculations. Adsorption, 2018, 24, 443-458.	3.0	12
25	Electronic structure tuning of stanene monolayers from DFT calculations: Effects of substitutional elemental doping. Applied Surface Science, 2018, 456, 290-301.	6.1	38
26	Adsorption of toxic SOx molecules on heterostructured TiO2/ZnO nanocomposites for gas sensing applications: a DFT study. Adsorption, 2018, 24, 29-41.	3.0	17
27	Adsorption and dissociation of H2S on nitrogen-doped TiO2 anatase nanoparticles: Insights from DFT computations. Surfaces and Interfaces, 2017, 8, 15-27.	3.0	16
28	Adsorption and dissociation of SO 3 on N-doped TiO 2 supported Au overlayers investigated by van der Waals corrected DFT. Surface Science, 2017, 663, 35-46.	1.9	10
29	A novel strategy for SO x removal by N-doped TiO 2 /WSe 2 nanocomposite as a highly efficient molecule sensor investigated by van der Waals corrected DFT. Computational and Theoretical Chemistry, 2017, 1114, 8-19.	2.5	30
30	A novel nitrogen dioxide gas sensor based on TiO2-supported Au nanoparticles: a van der Waals corrected DFT study. Journal of Nanostructure in Chemistry, 2017, 7, 121-132.	9.1	16
31	An innovative gas sensor system designed from a sensitive nanostructured ZnO for the selective detection of SO_x molecules: a density functional theory study. New Journal of Chemistry, 2017, 41, 12569-12580.	2.8	58
32	Density functional theory (DFT) study of O3 molecules adsorbed on nitrogen-doped TiO2/MoS2 nanocomposites: applications to gas sensor devices. Journal of the Iranian Chemical Society, 2017, 14, 2615-2626.	2.2	2
33	Prediction of a highly sensitive molecule sensor for SO_x detection based on TiO₂/MoS₂ nanocomposites: a DFT study. Journal of Sulfur Chemistry, 2017, 38, 52-68.	2.0	36
34	Molecular design of O3 and NO2 sensor devices based on a novel heterostructured N-doped TiO2/ZnO nanocomposite: a van der Waals corrected DFT study. Journal of Nanostructure in Chemistry, 2017, 7, 345-358.	9.1	17
35	Modified N-doped TiO 2 anatase nanoparticle as an ideal O 3 gas sensor: Insights from density functional theory calculations. Computational and Theoretical Chemistry, 2016, 1095, 15-28.	2.5	29
36	Theoretical study of the adsorption of NOx on TiO2/MoS2 nanocomposites: a comparison between undoped and N-doped nanocomposites. Journal of Nanostructure in Chemistry, 2016, 6, 309-327.	9.1	27

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37	Chemisorption of CH 2 O on N-doped TiO 2 anatase nanoparticle as modified nanostructure media: A DFT study. Surface Science, 2016, 654, 20-32.	1.9	12
38	N-doped TiO₂ anatase nanoparticles as a highly sensitive gas sensor for NO₂ detection: insights from DFT computations. Environmental Science: Nano, 2016, 3, 1153-1164.	4.3	83
39	Improving the adsorption of sulfur trioxide on TiO2 anatase nanoparticles by N-doping: A DFT study. Journal of Theoretical and Computational Chemistry, 2015, 14, 1550025.	1.8	5