

Ali Shokuhi Rad

List of Publications by Year in descending order

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57631

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docs citations

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#	ARTICLE	IF	CITATIONS
1	Study of the adsorption of chloropicrin on pure and Ga and Al doped B ₁₂ N ₁₂ : a comprehensive DFT and QTAIM investigation. <i>Molecular Simulation</i> , 2022, 48, 776-788.	0.9	16
2	DFT Study of Adsorption of Methyl Red on the Surface of Pure, Pyrrolidine-Functionalized, Silicon- and Germanium-Doped Zigzag (6, 0) Carbon Nanotubes. <i>Russian Journal of Physical Chemistry A</i> , 2022, 96, 1280-1290.	0.1	2
3	The computational quantum mechanical study of sulfamide drug adsorption onto X ₁₂ Y ₁₂ fullerene-like nanocages: detailed DFT and QTAIM investigations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 5427-5437.	2.0	59
4	Potential of graphene oxide as a drug delivery system for Sumatriptan: a detailed density functional theory study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 1611-1620.	2.0	30
5	Investigations of adsorption behavior and anti-inflammatory activity of glycine functionalized Al ₁₂ N ₁₂ and Al ₁₂ ON ₁₁ fullerene-like cages. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 119023.	2.0	23
6	DFT calculations towards the geometry optimization, electronic structure, infrared spectroscopy and UV-vis analyses of Favipiravir adsorption on the first-row transition metals doped fullerenes; a new strategy for COVID-19 therapy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 247, 119082.	2.0	72
7	Are nickel- and titanium- doped fullerenes suitable adsorbents for dopamine in an aqueous solution? Detailed DFT and AIM studies. <i>Journal of Molecular Liquids</i> , 2021, 322, 114942.	2.3	28
8	Conformational analysis and DFT investigations of two triazole derivatives and its halogenated substitution by using spectroscopy, AIM and Molecular docking. <i>Chemical Data Collections</i> , 2021, 31, 100625.	1.1	16
9	Synthesis of Fe ₃ O ₄ @chitosan@ZIF-8 towards removal of malachite green from aqueous solution: Theoretical and experimental studies. <i>International Journal of Biological Macromolecules</i> , 2021, 168, 428-441.	3.6	44
10	Reduced frequency of T helper 17 and T helper 1 cells and their association with critical coronavirus disease 2019. <i>Apmis</i> , 2021, 129, 271-279.	0.9	8
11	Response Surface Methodology Towards Optimization of Calotropis Procera Essential Oil Extraction by Using Supercritical CO ₂ . <i>Natural Products Journal</i> , 2021, 11, 97-107.	0.1	0
12	Theoretical investigation on the reactive and interaction properties of sorafenib – DFT, AIM, spectroscopic and Hirshfeld analysis, docking and dynamics simulation. <i>Journal of Molecular Liquids</i> , 2021, 330, 115652.	2.3	34
13	Gelatin-coated gold nanoparticles as an effective pH-sensitive methotrexate drug delivery system for breast cancer treatment. <i>Materials Today Chemistry</i> , 2021, 20, 100474.	1.7	33
14	MD, DFT Investigations and Inhibition of the Novel SARS- CoV-2 Mainprotease in Three Cocrystals of Hydrochloro- thiazide. <i>Analytical Chemistry Letters</i> , 2021, 11, 450-468.	0.4	3
15	Spectroscopic and computational study of chromone derivatives with antitumor activity: detailed DFT, QTAIM and docking investigations. <i>SN Applied Sciences</i> , 2021, 3, 1.	1.5	5
16	Enhancement in the mechanical property of NBR/PVC nanocomposite by using sulfur and electron beam curing in the presence of Cloisite 30B nanoclay. <i>Journal of Macromolecular Science - Pure and Applied Chemistry</i> , 2020, 57, 123-130.	1.2	4
17	Bovine serum albumin/gold nanoparticles as a drug delivery system for Curcumin: experimental and computational studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 4644-4654.	2.0	15
18	Conformational analysis and quantum descriptors of two new imidazole derivatives by experimental, DFT, AIM, molecular docking studies and adsorption activity on graphene. <i>Heliyon</i> , 2020, 6, e05182.	1.4	16

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19	Synthesis of cellulose nanofibers functionalized by dithiooxamide for preconcentration and determination of trace amounts of Cd(II) ions in water samples. <i>Cellulose</i> , 2020, 27, 8885-8898.	2.4	21
20	Computational investigation of the strategy of DNA/RNA stabilization through the study of the conjugation of an oligonucleotide with silver and gold nanoparticles. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5690.	1.7	11
21	Synthesis of Grafted Nanofibrillated Cellulose-Based Hydrogel and Study of Its Thermodynamic, Kinetic, and Electronic Properties. <i>Journal of Agricultural and Food Chemistry</i> , 2020, 68, 8710-8719.	2.4	39
22	The morphological properties and biocompatibility studies of synthesized nanocomposite foam from modified polyethersulfone/graphene oxide using supercritical CO ₂ . <i>Journal of Macromolecular Science - Pure and Applied Chemistry</i> , 2020, 57, 451-460.	1.2	16
23	Conjugation of pectin biopolymer with Au nanoparticles as a drug delivery system: Experimental and DFT studies. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5609.	1.7	26
24	Corrosion control of aluminum in the solutions of NaCl, HCl and NaOH using 2,6-dimethylpyridine inhibitor: Experimental and DFT insights. <i>Materials Chemistry and Physics</i> , 2020, 244, 122681.	2.0	46
25	Synthesis and application of chitosan/tripolyphosphate/graphene oxide hydrogel as a new drug delivery system for Sumatriptan Succinate. <i>Journal of Molecular Liquids</i> , 2020, 315, 113835.	2.3	59
26	Supercritical Extraction of <i>Heracleum persicum</i> Plant and Mathematical Modeling. <i>Natural Products Journal</i> , 2020, 10, 298-311.	0.1	0
27	Removal of Bismuth (III) ions from water solution using a cellulose-based nanocomposite: A detailed study by DFT and experimental insights. <i>Journal of Molecular Liquids</i> , 2019, 295, 111723.	2.3	25
28	Calcium-doped single-wall nanotubes (Ca/SWCNTs) as a superior carrier for atropine drug delivery: a quantum-chemical study in gas and solvent phases. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 4267-4273.	2.0	16
29	X ₁₂ N ₁₂ (X=Al, B) clusters for protection of vitamin C; molecular modeling investigation. <i>Surfaces and Interfaces</i> , 2019, 15, 30-37.	1.5	38
30	Change in the electronic and nonlinear optical properties of Fullerene through its incorporation with Sc-, Fe-, Cu-, and Zn transition metals. <i>Applied Physics A: Materials Science and Processing</i> , 2019, 125, 1.	1.1	26
31	Functionalization of SBA-15 by dithiooxamide towards removal of Co (II) ions from real samples: Isotherm, thermodynamic and kinetic studies. <i>Advanced Powder Technology</i> , 2019, 30, 1823-1834.	2.0	18
32	Gelatin-Gold Nanoparticles as an Ideal Candidate for Curcumin Drug Delivery: Experimental and DFT Studies. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2019, 29, 2186-2196.	1.9	23
33	Experimental and computational studies on the synthesis of diastereoselective natural-based Meldrum spiro dibenzofuran derivatives. <i>New Journal of Chemistry</i> , 2019, 43, 6615-6621.	1.4	6
34	Dispersive liquid-liquid microextraction based on green type solvents "deep eutectic solvents" for highly selective separation and efficient preconcentration of nickel in water samples. <i>Journal of the Iranian Chemical Society</i> , 2019, 16, 1715-1722.	1.2	24
35	A theoretical study of two novel Schiff bases as inhibitors of carbon steel corrosion in acidic medium. <i>Applied Physics A: Materials Science and Processing</i> , 2019, 125, 1.	1.1	25
36	A Comparative Computational Investigation of Phosgene Adsorption on (XY) ₁₂ (X=Al, B and Y=N, P) Nanoclusters: DFT Investigations. <i>Journal of Cluster Science</i> , 2019, 30, 203-218.	1.7	34

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37	Quantitative and Qualitative Analyses of Genus Pyrus L. (Pear Tree) in West Azerbaijan Province, Iran. Iranian Journal of Science and Technology, Transaction A: Science, 2019, 43, 715-724.	0.7	1
38	Fabrication of TFC nanofiltration membranes via co-solvent assisted interfacial polymerization for lactose recovery. Arabian Journal of Chemistry, 2019, 12, 5325-5338.	2.3	23
39	How can nickel decoration affect H ₂ adsorption on B ₁₂ P ₁₂ nano-heterostructures?. Journal of Molecular Liquids, 2018, 255, 168-175.	2.3	50
40	Comparison of X ₁₂ Y ₁₂ (X=Al, B and Y=N, P) fullerene-like nanoclusters toward adsorption of dimethyl ether. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850013.	1.8	23
41	Impacts of zeolite nanoparticles on substrate properties of thin film nanocomposite membranes for engineered osmosis. Journal of Nanoparticle Research, 2018, 20, 1.	0.8	42
42	Functionalization of (n, 0) CNTs (n = 3-16) by uracil: DFT studies. European Physical Journal B, 2018, 91, 1.	0.6	7
43	Adsorption of acid blue on synthesized polymeric nanocomposites, PPy/MCM-41 and PANi/MCM-41: Isotherm, thermodynamic and kinetic studies. Journal of Macromolecular Science - Pure and Applied Chemistry, 2018, 55, 269-279.	1.2	21
44	Potential of Advanced Nano-structured Membranes for Landfill Leachate Treatment: A Review. ChemBioEng Reviews, 2018, 5, 119-138.	2.6	17
45	Surface interaction of H ₂ O and H ₂ S onto Ca ₁₂ O ₁₂ nanocluster: Quantum-chemical analyses. Surface and Interface Analysis, 2018, 50, 411-419.	0.8	47
46	Strengthening of polysulfone membranes using hybrid mixtures of micro- and nano-scale modifiers. Frontiers of Chemical Science and Engineering, 2018, 12, 174-183.	2.3	15
47	PVDF membrane assisted by modified hydrophobic ZnO nanoparticle for membrane distillation. Asia-Pacific Journal of Chemical Engineering, 2018, 13, e2196.	0.8	38
48	Dispersive liquid-liquid microextraction using the freeze floating organic drop for rapid, fast, and sensitive determination of lead. International Journal of Environmental Analytical Chemistry, 2018, 98, 247-257.	1.8	8
49	Esterification of Waste Chicken Fat: Sulfonated MWCNT Toward Biodiesel Production. Waste and Biomass Valorization, 2018, 9, 591-599.	1.8	27
50	Determination of Compositions of Thymus Pubescens; the Comparison of Different Solvents Towards Extraction. Iranian Journal of Science and Technology, Transaction A: Science, 2018, 42, 1923-1928.	0.7	6
51	Effects of perlite and caustic soda on microorganism activities of leachate in a sequence batch reactor. Environmental Technology (United Kingdom), 2018, 39, 2321-2334.	1.2	10
52	Application of chromium-doped fullerene as a carrier for thymine and uracil nucleotides: Comprehensive density functional theory calculations. Applied Organometallic Chemistry, 2018, 32, e4070.	1.7	27
53	Nonlinear optical and electronic properties of Cr-, Ni-, and Ti-substituted C ₂₀ fullerenes: A quantum-chemical study. Materials Research Bulletin, 2018, 97, 399-404.	2.7	91
54	Potential of metal-fullerene hybrids as strong nanocarriers for cytosine and guanine nucleobases: A detailed DFT study. Current Applied Physics, 2018, 18, 133-140.	1.1	33

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55	Application of SBA-15/Diphenyl Carbazon/SDS Nanocomposite as Solid-Phase Extractor for Simultaneous Determination of Cu(II) and Zn(II) Ions. Arabian Journal for Science and Engineering, 2018, 43, 3547-3556.	1.7	18
56	Chemically uracil-functionalized carbon and silicon carbide nanotubes: Computational studies. Materials Chemistry and Physics, 2018, 205, 164-170.	2.0	12
57	Sublayer assisted by hydrophilic and hydrophobic ZnO nanoparticles toward engineered osmosis process. Korean Journal of Chemical Engineering, 2018, 35, 2256-2268.	1.2	18
58	Beryllium oxide (BeO) nanotube provides excellent surface towards adenine adsorption: A dispersion-corrected DFT study in gas and water phases. Current Applied Physics, 2018, 18, 1059-1065.	1.1	56
59	Is it possible to use $X_{12}Y_{12}$ ($X = Al, B,$ and $Y = N, P$) nanocages for drug-delivery systems? A DFT study on the adsorption property of 4-aminopyridine drug. Applied Physics A: Materials Science and Processing, 2018, 124, 1.	1.1	54
60	Preparation of magnetic nanocomposite based on polyaniline/Fe ₃ O ₄ towards removal of lead (II) ions from real samples. Synthetic Metals, 2018, 245, 1-9.	2.1	43
61	Three-component solventless Strecker synthesis of α -aminonitriles catalysed by a renewable sulfonated nanoporous carbon catalyst (CMK-5O ₃ H). Applied Organometallic Chemistry, 2018, 32, e4422.	1.7	8
62	Nonlinear optical, IR and orbital properties of Ni doped MgO nanoclusters: A DFT investigation. Computational and Theoretical Chemistry, 2018, 1138, 39-47.	1.1	21
63	DFT study of boron trichloride adsorption on the surface of Al ₁₂ N ₁₂ nanocluster. Molecular Physics, 2017, 115, 879-884.	0.8	24
64	Application of B ₁₂ N ₁₂ and B ₁₂ P ₁₂ as two fullerene-like semiconductors for adsorption of halomethane: Density functional theory study. Semiconductors, 2017, 51, 134-138.	0.2	18
65	Nickel-decorated B ₁₂ P ₁₂ nanoclusters as a strong adsorbent for SO ₂ adsorption: Quantum chemical calculations. Canadian Journal of Physics, 2017, 95, 958-962.	0.4	44
66	Adsorption of thiophene on the surfaces of $X_{12}Y_{12}$ ($X = Al, B,$ and $Y = N, P$) nanoclusters; A DFT study. Journal of Molecular Liquids, 2017, 238, 303-309.	2.3	88
67	DFT studies of stabilities and properties for $X_3Y_6Z_9$ borazine-like structures ($X = B/Al, Y = N/P, Z = H/Me$). Superlattices and Microstructures, 2017, 109, 360-365.	1.4	4
68	Sulfonic acid supported on magnetic nanoparticle as an eco-friendly, durable and robust catalyst for the synthesis of α -amino carbonyl compounds through solvent free Mannich reaction. Applied Organometallic Chemistry, 2017, 31, e3865.	1.7	12
69	A new route of bioaugmentation by allochthonous and autochthonous through biofilm bacteria for soluble chemical oxygen demand removal of old leachate. Environmental Technology (United Tj ETQq1 1 0.784314.ogBT /Overlock 10 T		
70	Developing PES membrane by modified Co ₃ O ₄ -OA nanoparticles for direct contact membrane distillation process. Asia-Pacific Journal of Chemical Engineering, 2017, 12, 582-594.	0.8	10
71	O ₃ and SO ₂ sensing concept on extended surface of B ₁₂ N ₁₂ nanocages modified by Nickel decoration: A comprehensive DFT study. Solid State Sciences, 2017, 69, 22-30.	1.5	87
72	Adsorption photobioreactor as a co-treatment system for ammonium and phosphate removal by the response surface method. Waste Management and Research, 2017, 35, 766-775.	2.2	4

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73	Preparation of Modified MWCNT with Dithiooxamide for Preconcentration and Determination of Trace Amounts of Cobalt Ions in Food and Natural Water Samples. <i>ChemistrySelect</i> , 2017, 2, 4439-4444.	0.7	12
74	Application of pristine and Ni-decorated B ₁₂ P ₁₂ nano-clusters as superior media for acetylene and ethylene adsorption: DFT calculations. <i>Computational and Theoretical Chemistry</i> , 2017, 1109, 1-9.	1.1	69
75	Adsorption properties of acetylene and ethylene molecules onto pristine and nickel-decorated Al ₁₂ N ₁₂ nanoclusters. <i>Materials Chemistry and Physics</i> , 2017, 194, 337-344.	2.0	55
76	Quantum Chemical Study on the adsorption of metformin drug on the surface of pristine, Si- and Al-doped (5, 5) SWCNTs. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2017, 90, 204-213.	1.3	47
77	Sulfur mustard gas adsorption on ZnO fullerene-like nanocage: Quantum chemical calculations. <i>Superlattices and Microstructures</i> , 2017, 106, 122-128.	1.4	66
78	DFT study on the adsorption of diethyl, ethyl methyl, and dimethyl ethers on the surface of gallium doped graphene. <i>Applied Surface Science</i> , 2017, 401, 156-161.	3.1	44
79	Study of dimethyl ester interaction on the surface of Ga-doped graphene: Application of density functional theory. <i>Journal of Molecular Liquids</i> , 2017, 229, 1-5.	2.3	16
80	Substitutional doping of zirconium-, molybdenum-, ruthenium-, and palladium: An effective method to improve nonlinear optical and electronic property of C ₂₀ fullerene. <i>Computational and Theoretical Chemistry</i> , 2017, 1121, 68-75.	1.1	37
81	A DFT study of O ₂ and Cl ₂ adsorption onto Al ₁₂ N ₁₂ fullerene-like nanocluster. <i>Heteroatom Chemistry</i> , 2017, 28, .	0.4	18
82	Surface interaction of H ₂ S, SO ₂ , and SO ₃ on fullerene-like gallium nitride (GaN) nanostructure semiconductor. <i>Solid State Communications</i> , 2017, 265, 6-11.	0.9	19
83	Nickel Based Paddle-Wheel Metal-Organic Frameworks Towards Adsorption of O ₃ and SO ₂ Molecules: Quantum-Chemical Calculations. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2017, 27, 1826-1834.	1.9	12
84	Preparation of SBA-15/graphene oxide nanocomposites for preconcentration and determination of trace amounts of rutoside in blood plasma and urine. <i>Sensors and Actuators B: Chemical</i> , 2017, 253, 533-541.	4.0	19
85	Improving the Mechanical Performance and Thermal Stability of a PVA-Clay Nanocomposite by Electron Beam Irradiation. <i>Mechanics of Composite Materials</i> , 2017, 53, 373-380.	0.9	6
86	High ozone chemisorption by using metal-cluster complexes: a DFT study on the nickel-decorated B ₁₂ P ₁₂ nanoclusters. <i>Canadian Journal of Chemistry</i> , 2017, 95, 845-850.	0.6	15
87	Study on the electronic structure of Cr- and Ni-doped fullerenes upon adsorption of adenine: A comprehensive DFT calculation. <i>Diamond and Related Materials</i> , 2017, 77, 116-121.	1.8	65
88	Chemisorption of BH ₃ and BF ₃ on aluminum nitride nanocluster: quantum-chemical investigations. <i>Journal of Nanostructure in Chemistry</i> , 2017, 7, 207-215.	5.3	13
89	Anti-bacterial assay of doped membrane by zero valent Fe nanoparticle via in-situ and ex-situ aspect. <i>Chemical Engineering Research and Design</i> , 2017, 117, 287-300.	2.7	29
90	Surface modification of mesoporous silicate by tannin for immobilization of TiO ₂ nanoparticles: Study of photocatalytic performance. <i>Materials Chemistry and Physics</i> , 2017, 185, 14-23.	2.0	7

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91	Synthesis of Magnetite Nanoparticles by Biological Technique. Biosciences, Biotechnology Research Asia, 2017, 14, 631-633.	0.2	4
92	Functionalization of MWCNT by "SO ₃ H and "COOH Groups and Their Application as Solid Acidic Catalysts for Esterification of Waste Chicken Fat. Chemical and Biochemical Engineering Quarterly, 2017, 31, 69-75.	0.5	3
93	Performance and modeling of a moving bed biofilm process: nickel and chromium heavy metal removal from industrial wastewater. RSC Advances, 2016, 6, 113737-113744.	1.7	10
94	Extraction of Eugenol from Carnation: A Quantitative and Qualitative Analysis by Aqueous and Ethanolic Solvents. Journal of Essential Oil-bearing Plants: JEOP, 2016, 19, 1495-1502.	0.7	6
95	Comparative experimental study on fouling mechanisms in nano-porous membrane: cheese whey ultrafiltration as a case study. Water Science and Technology, 2016, 74, 2737-2750.	1.2	14
96	Density functional theory study of the adsorption of MeOH and EtOH on the surface of Pt-decorated graphene. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 83, 135-140.	1.3	48
97	Study on the structure and electronic property of adsorbed guanine on aluminum doped graphene: First principles calculations. Current Applied Physics, 2016, 16, 527-533.	1.1	70
98	Mathematical modeling of continuous ethanol fermentation in a membrane bioreactor by pervaporation compared to conventional system: Genetic algorithm. Bioresource Technology, 2016, 212, 62-71.	4.8	24
99	Ab-Initio Study of Physisorption of Hydrogen Cyanide on 2PANI: a Model for Polyaniline Gas Sensor. Zeitschrift Fur Physikalische Chemie, 2016, 230, 1487-1498.	1.4	12
100	First-principles DFT study of SO ₂ and SO ₃ adsorption on 2PANI: a model for polyaniline response. Journal of Sulfur Chemistry, 2016, 37, 622-631.	1.0	28
101	The polythiophene molecular segment as a sensor model for H ₂ O, HCN, NH ₃ , SO ₃ , and H ₂ S: a density functional theory study. Journal of Molecular Modeling, 2016, 22, 127.	0.8	20
102	Adsorption of mercaptopyridine on the surface of Al- and B-doped graphenes: Theoretical study. Journal of Alloys and Compounds, 2016, 682, 345-351.	2.8	58
103	Study on the surface interaction of Furan with X ₁₂ Y ₁₂ (X=Al, P) semiconductors: DFT calculations. Heteroatom Chemistry, 2016, 27, 316-322.	0.4	51
104	DFT study of hydrogen fluoride and sulfur trioxide interactions on the surface of Pt-decorated graphene. Iranian Physical Journal, 2016, 10, 307-313.	1.2	15
105	Enhancement in hydrogen molecule adsorption on B ₁₂ N ₁₂ nano-cluster by decoration of nickel. International Journal of Hydrogen Energy, 2016, 41, 22182-22191.	3.8	100
106	Theoretical study of chemisorption of cyanuric fluoride and S-triazine on the surface of Al-doped graphene. Molecular Simulation, 2016, 42, 1519-1527.	0.9	15
107	Coordination of nickel atoms with Al ₁₂ X ₁₂ (X=Al, P) nanocages enhances H ₂ adsorption: A surface study by DFT. Vacuum, 2016, 133, 70-80.	1.6	67
108	Surface study of gallium- and aluminum- doped graphenes upon adsorption of cytosine: DFT calculations. Applied Surface Science, 2016, 390, 444-451.	3.1	48

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109	Acid-treated zeolite (clinoptilolite) and its potential to zinc removal from water sample. International Journal of Environmental Science and Technology, 2016, 13, 2705-2712.	1.8	12
110	Study on the electronic structure of Al ₁₂ N ₁₂ and Al ₁₂ P ₁₂ fullerene-like nano-clusters upon adsorption of CH ₃ F and CH ₃ Cl. Molecular Physics, 2016, 114, 3143-3149.	0.8	47
111	Surface study of platinum decorated graphene towards adsorption of NH ₃ and CH ₄ . Materials Chemistry and Physics, 2016, 182, 32-38.	2.0	50
112	Adsorption of adenine on the surface of nickel-decorated graphene; A DFT study. Journal of Alloys and Compounds, 2016, 686, 662-668.	2.8	66
113	Adsorption of pyrrole on Al ₁₂ N ₁₂ , Al ₁₂ P ₁₂ , B ₁₂ N ₁₂ , and B ₁₂ P ₁₂ fullerene-like nano-cages; a first principles study. Vacuum, 2016, 131, 135-141.	1.6	83
114	Detailed surface study of adsorbed nickel on Al ₁₂ N ₁₂ nano-cage. Thin Solid Films, 2016, 612, 179-185.	0.8	55
115	Adsorption properties of SO ₂ and O ₃ molecules on Pt-decorated graphene: A theoretical study. Vacuum, 2016, 130, 113-118.	1.6	117
116	Application of carbon nanostructures toward SO ₂ and SO ₃ adsorption: a comparison between pristine graphene and N-doped graphene by DFT calculations. Journal of Sulfur Chemistry, 2016, 37, 176-188.	1.0	129
117	Adsorption of C ₂ H ₂ and C ₂ H ₄ on Pt-decorated graphene nanostructure: Ab-initio study. Synthetic Metals, 2016, 211, 115-120.	2.1	77
118	Ni adsorption on Al ₁₂ P ₁₂ nano-cage: A DFT study. Journal of Alloys and Compounds, 2016, 678, 317-324.	2.8	102
119	A comparative density functional theory study of guanine chemisorption on Al ₁₂ N ₁₂ , Al ₁₂ P ₁₂ , B ₁₂ N ₁₂ , and B ₁₂ P ₁₂ nano-cages. Journal of Alloys and Compounds, 2016, 672, 161-169.	2.8	151
120	Study on the adsorption properties of O ₃ , SO ₂ , and SO ₃ on B-doped graphene using DFT calculations. Journal of Solid State Chemistry, 2016, 237, 204-210.	1.4	156
121	Terthiophene as a model sensor for some atmospheric gases: theoretical study. Molecular Physics, 2016, 114, 584-591.	0.8	19
122	N-doped graphene as a nanostructure adsorbent for carbon monoxide: DFT calculations. Molecular Physics, 2016, 114, 1756-1762.	0.8	69
123	Chemisorption of NO on Pt-decorated graphene as modified nanostructure media: A first principles study. Applied Surface Science, 2016, 360, 1041-1046.	3.1	145
124	Synthesis of polyaniline/Fe ₃ O ₄ magnetic nanoparticles for removal of reactive red 198 from textile waste water: kinetic, isotherm, and thermodynamic studies. Desalination and Water Treatment, 2016, 57, 22551-22563.	1.0	38
125	Al-doped graphene as a new nanostructure adsorbent for some halomethane compounds: DFT calculations. Surface Science, 2016, 645, 6-12.	0.8	95
126	Use of Modified ¹³ Alumina Nanoparticles for the Extraction and Preconcentration of Trace Amounts of Cadmium Ions. Australian Journal of Chemistry, 2016, 69, 314.	0.5	16

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127	Density functional study of Al-doped graphene nanostructure towards adsorption of CO, CO ₂ and H ₂ O. <i>Synthetic Metals</i> , 2015, 210, 171-178.	2.1	103
128	Preparation of modified magnetic nanoparticles as a sorbent for the preconcentration and determination of cadmium ions in food and environmental water samples prior to flame atomic absorption spectrometry. <i>Journal of Magnetism and Magnetic Materials</i> , 2015, 381, 138-144.	1.0	57
129	Adsorption of acetyl halide molecules on the surface of pristine and Al-doped graphene: Ab initio study. <i>Applied Surface Science</i> , 2015, 355, 233-241.	3.1	91
130	Ab-initio study of interaction of some atmospheric gases (SO ₂ , NH ₃ , H ₂ O, CO, CH ₄ and CO ₂) with polypyrrole (3PPy) gas sensor: DFT calculations. <i>Sensors and Actuators B: Chemical</i> , 2015, 220, 641-651.	4.0	107
131	Modified surface based on magnetic nanocomposite of dithiooxamide/Fe ₃ O ₄ as a sorbent for preconcentration and determination of trace amounts of copper. <i>Journal of Magnetism and Magnetic Materials</i> , 2015, 389, 130-135.	1.0	27
132	Interaction of SO ₂ and SO ₃ on terthiophene (as a model of polythiophene gas sensor): DFT calculations. <i>Chemical Physics Letters</i> , 2015, 639, 29-35.	1.2	62
133	First principles study of Al-doped graphene as nanostructure adsorbent for NO ₂ and N ₂ O: DFT calculations. <i>Applied Surface Science</i> , 2015, 357, 1217-1224.	3.1	189
134	Interaction of methanol with some aniline and pyrrole derivatives: DFT calculations. <i>Synthetic Metals</i> , 2015, 209, 502-511.	2.1	44
135	Application of modified magnetic nanoparticles as a sorbent for preconcentration and determination of nickel ions in food and environmental water samples. <i>TrAC - Trends in Analytical Chemistry</i> , 2015, 74, 146-151.	5.8	40
136	First-principles study of terpyrrole as a potential hydrogen cyanide sensor: DFT calculations. <i>Journal of Molecular Modeling</i> , 2015, 21, 273.	0.8	44
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