Mohammad Ghashghaee

List of Publications by Year
in descending order

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63 papers	1,453 citations	257450 24 h-index	414414 32 g-index
63 all docs	63 docs citations	63 times ranked	787 citing authors

#	Article	IF	Citations
1	Scandium doping of black phosphorene for enhanced sensitivity to hydrogen sulfide: Periodic DFT calculations. Journal of Physics and Chemistry of Solids, 2021, 148, 109765.	4.0	14
2	Detection of CNX cyanogen halides (Xâ€‰=â€‰F, Cl) on metal-free defective phosphorene sensor: periodic DFT calculations. Molecular Physics, 2021, 119, e1819577.	1.7	17
3	Alkali metal doping of black phosphorus monolayer for ultrasensitive capture and detection of nitrogen dioxide. Scientific Reports, 2021, 11, 842.	3.3	9
4	Molecular-level insights into adsorption of a novel silyl ester donor on essential MgCl2 facets of supported Zieglerâ€“Natta catalysts. Journal of Physics and Chemistry of Solids, 2021, 159, 110249.	4.0	3
5	Theoretical insights into sensing of hexavalent chromium on buckled and planar polymeric carbon nitride nanosheets of heptazine and triazine structures. Molecular Simulation, 2020, 46, 54-61.	2.0	28
6	Adsorption of iron(II, III) cations on pristine heptazine and triazine polymeric carbon nitride quantum dots of buckled and planar structures: theoretical insights. Adsorption, 2020, 26, 429-442.	3.0	32
7	Influence of NiO decoration on adsorption capabilities of black phosphorus monolayer toward nitrogen dioxide: periodic DFT calculations. Molecular Simulation, 2020, 46, 1062-1072.	2.0	31
8	Defective phosphorene for highly efficient formaldehyde detection: Periodic density functional calculations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126792.	2.1	29
9	Highly improved carbon dioxide sensitivity and selectivity of black phosphorene sensor by vacancy doping: A <scp>quantum chemical</scp> perspective. International Journal of Quantum Chemistry, 2020, 120, e26265.	2.0	24
10	Defect engineering and zinc oxide doping of black phosphorene for nitrogen dioxide capture and detection: quantum-chemical calculations. Applied Surface Science, 2020, 523, 146527.	6.1	37
11	Hydrogen detection on black phosphorene doped with Ni, Pd, and Pt: Periodic density functional calculations. International Journal of Hydrogen Energy, 2020, 45, 16298-16309.	7.1	35
12	Theoretical insights into hydrogen sensing capabilities of black phosphorene modified through ZnO doping and decoration. International Journal of Hydrogen Energy, 2020, 45, 16918-16928.	7.1	35
13	Remarkable improvement in phosgene detection with a defect-engineered phosphorene sensor: first-principles calculations. Physical Chemistry Chemical Physics, 2020, 22, 9677-9684.	2.8	36
14	Mn-Doped black phosphorene for ultrasensitive hydrogen sulfide detection: periodic DFT calculations. Physical Chemistry Chemical Physics, 2020, 22, 15549-15558.	2.8	26
15	Conductivity tuning of charged triazine and heptazine graphitic carbon nitride (g-C3N4) quantum dots via nonmetal (B, O, S, P) doping: DFT calculations. Journal of Physics and Chemistry of Solids, 2020, 141, 109422.	4.0	46
16	Quantum-chemical calculations on graphitic carbon nitride (g-C3N4) single-layer nanostructures: polymeric slab vs. quantum dot. Structural Chemistry, 2020, 31, 1137-1148.	2.0	22
17	Phosphorene defects for high-quality detection of nitric oxide and carbon monoxide: A periodic density functional study. Chemical Engineering Journal, 2020, 396, 125247.	12.7	36
18	Substitutional doping of black phosphorene with boron, nitrogen, and arsenic for sulfur trioxide detection: a theoretical perspective. Journal of Sulfur Chemistry, 2020, 41, 399-420.	2.0	27

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19	Functionalization and Doping of Black Phosphorus. Engineering Materials, 2020, , 1-30.	0.6	11
20	Chemistry of Black Phosphorus. Engineering Materials, 2020, , 59-72.	0.6	12
21	Future Prospects and Challenges of Black Phosphorous Materials. Engineering Materials, 2020, , 157-169.	0.6	10
22	Catalytic Degradation of Linear Low-Density Polyethylene Over USY Catalyst: Effect of Catalyst to Polymer Ratio. , 2020, , 511-514.		0
23	Adsorption of toxic mercury, lead, cadmium, and arsenic ions on black phosphorous nanosheet: first-principles calculations. Structural Chemistry, 2019, 30, 85-96.	2.0	31
24	Kinetics of different bioreactor systems with Acidithiobacillus ferrooxidans for ferrous iron oxidation. Reaction Kinetics, Mechanisms and Catalysis, 2019, 128, 611-627.	1.7	4
25	Superhydrophobic nanocomposite coatings of poly(methyl methacrylate) and stearic acid grafted CuO nanoparticles with photocatalytic activity. Progress in Organic Coatings, 2019, 136, 105270.	3.9	31
26	Synergistic Coconversion of Refinery Fuel Oil and Methanol over H-ZSM-5 Catalyst for Enhanced Production of Light Olefins. Energy & Fuels, 2019, 33, 5761-5765.	5.1	19
27	Dual role of ferric chloride in modification of USY catalyst for enhanced olefin production from refinery fuel oil. Applied Catalysis A: General, 2019, 580, 131-139.	4.3	10
28	Two-stage thermocatalytic upgrading of fuel oil to olefins and fuels over a nanoporous hierarchical acidic catalyst. Petroleum Science and Technology, 2019, 37, 1910-1916.	1.5	6
29	Structural diversity of metallacycle intermediates for ethylene dimerization on heterogeneous NiMCM-41 catalyst: a quantum chemical perspective. Structural Chemistry, 2019, 30, 137-150.	2.0	36
30	Steam catalytic cracking of fuel oil over a novel composite nanocatalyst: Characterization, kinetics and comparative perspective. Journal of Analytical and Applied Pyrolysis, 2019, 138, 281-293.	5.5	20
31	Molecular-level insights into furfural hydrogenation intermediates over single-atomic Cu catalysts on magnesia and silica nanoclusters. Molecular Simulation, 2019, 45, 154-163.	2.0	30
32	Catalytic transformation of ethylene to propylene and butene over an acidic Ca-incorporated composite nanocatalyst. Applied Catalysis A: General, 2019, 569, 20-27.	4.3	11
33	Thorough assessment of delayed coking correlations against literature data: Development of improved alternative models. Reaction Kinetics, Mechanisms and Catalysis, 2019, 126, 83-102.	1.7	9
34	Combined effect of nanoporous diluent and steam on catalytic upgrading of fuel oil to olefins and fuels over USY catalyst. Petroleum Science and Technology, 2018, 36, 750-755.	1.5	21
35	Methane adsorption and hydrogen atom abstraction at diatomic radical cation metal oxo clusters: first-principles calculations. Molecular Simulation, 2018, 44, 850-863.	2.0	18
36	Influence of catalyst additives on vapor-phase hydrogenation of furfural to furfuryl alcohol on impregnated copper/magnesia. Biomass Conversion and Biorefinery, 2018, 8, 79-86.	4.6	20

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37	Heterogeneous catalysts for gas-phase conversion of ethylene to higher olefins. Reviews in Chemical Engineering, 2018, 34, 595-655.	4.4	50
38	HYDROTALCITE-IMPREGNATED COPPER AND CHROMIUM-DOPED COPPER AS NOVEL AND EFFICIENT CATALYSTS FOR VAPOR-PHASE HYDROGENATION OF FURFURAL: EFFECT OF CLAY PRETREATMENT. Brazilian Journal of Chemical Engineering, 2018, 35, 669-678.	1.3	11
39	Ethene Protonation Over Silica-Grafted Metal (Cr, Mo, and W) Oxide Catalysts: A Comparative Nanocluster Modeling Study. Russian Journal of Inorganic Chemistry, 2018, 63, 1570-1577.	1.3	33
40	Spray-Deposition of an Organic/Inorganic Blend for Fabrication of a Superhydrophobic Surface: Effect of Admixing with Silica Aerogel and Modified Silica Nanoparticles. Protection of Metals and Physical Chemistry of Surfaces, 2018, 54, 909-916.	1.1	16
41	Initiation of heterogeneous Schrock-type Mo and W oxide metathesis catalysts: A quantum thermochemical study. Computational Materials Science, 2018, 155, 197-208.	3.0	31
42	Nanostructured Hydrotalcite-Supported RuBaK Catalyst for Direct Conversion of Ethylene to Propylene. Russian Journal of Applied Chemistry, 2018, 91, 972-976.	0.5	13
43	Two-Step Thermal Cracking of an Extra-Heavy Fuel Oil: Experimental Evaluation, Characterization, and Kinetics. Industrial & Engineering Chemistry Research, 2018, 57, 7421-7430.	3.7	41
44	A Novel Consecutive Approach for the Preparation of Cuâ€“MgO Catalysts with High Activity for Hydrogenation of Furfural to Furfuryl Alcohol. Catalysis Letters, 2017, 147, 318-327.	2.6	40
45	Preparation of Cu-MgO catalysts with different copper precursors and precipitating agents for the vapor-phase hydrogenation of furfural. Korean Journal of Chemical Engineering, 2017, 34, 692-700.	2.7	24
46	Effect of promoter on selective hydrogenation of furfural over Cu-Cr/TiO2 catalyst. Russian Journal of Applied Chemistry, 2017, 90, 304-309.	0.5	9
47	Kinetic models for hydroconversion of furfural over the ecofriendly Cu-MgO catalyst: An experimental and theoretical study. Applied Catalysis A: General, 2017, 545, 134-147.	4.3	55
48	Comment on â€˜hydrogen/methanol production in a novel multifunctional reactor with in situ adsorption: modeling and optimizationâ€™. International Journal of Energy Research, 2017, 41, 461-462.	4.5	0
49	Cluster modeling and coordination structures of Cu+ ions in Al-incorporated Cu-MEL catalysts â€“ a density functional theory study. Journal of the Mexican Chemical Society, 2017, 61, .	0.6	28
50	Diversity of monomeric dioxo chromium species in Cr/silicalite-2 catalysts: A hybrid density functional study. Computational Materials Science, 2016, 118, 147-154.	3.0	25
51	Theoretical identification of structural heterogeneities of divalent nickel active sites in NiMCM-41 nanoporous catalysts. Journal of Nanostructure in Chemistry, 2016, 6, 365-372.	9.1	21
52	Characterization of extraframework Zn2+ cationic sites in silicalite-2: a computational study. Structural Chemistry, 2016, 27, 467-475.	2.0	26
53	Removal of Cr(VI) Species from Aqueous Solution by Different Nanoporous Materials. Iranian Journal of Toxicology, 2016, 10, 15-21.	0.3	15
54	Saturated Five-membered N,B-Heterocyclic Carbene: A Computational Study. Chemistry Letters, 2015, 44, 1586-1588.	1.3	3

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55	Predictive correlations for thermal upgrading of petroleum residues. Journal of Analytical and Applied Pyrolysis, 2015, 115, 326-336.	5.5	22
56	Saturated N,X-Heterocyclic Carbenes (X=N, O, S, P, Si, C, and B): Stability, Nucleophilicity, and Basicity. Australian Journal of Chemistry, 2015, 68, 1438.	0.9	24
57	Comparison of four nanoporous catalysts in thermocatalytic upgrading of vacuum residue. Journal of Analytical and Applied Pyrolysis, 2013, 102, 97-102.	5.5	18
58	Applicability of protolytic mechanism to steady-state heterogeneous dehydrogenation of ethane revisited. Microporous and Mesoporous Materials, 2013, 170, 318-330.	4.4	21
59	Investigation of kinetics and cracked oil structural changes in thermal cracking of Iranian vacuum residues. Fuel Processing Technology, 2011, 92, 2226-2234.	7.2	49
60	Multivariable optimization of thermal cracking severity. Chemical Engineering Research and Design, 2011, 89, 1067-1077.	5.6	25
61	Evolutionary model for computation of pore-size distribution in microporous solids of cylindrical pore structure. Microporous and Mesoporous Materials, 2011, 138, 22-31.	4.4	10
62	Effect of Solvent Dearomatization and Operating Conditions in Steam Pyrolysis of a Heavy Feedstock. Energy & Fuels, 2010, 24, 1899-1907.	5.1	11
63	Flowsheeting of steam cracking furnaces. Chemical Engineering Research and Design, 2009, 87, 36-46.	5.6	46