

Mohammad Ghashghaee

List of Publications by Year in descending order

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63
papers

1,453
citations

293460

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docs citations

63
times ranked

882
citing authors

#	ARTICLE	IF	CITATIONS
1	Scandium doping of black phosphorene for enhanced sensitivity to hydrogen sulfide: Periodic DFT calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2021, 148, 109765.	1.9	14
2	Detection of CNX cyanogen halides (X = F, Cl) on metal-free defective phosphorene sensor: periodic DFT calculations. <i>Molecular Physics</i> , 2021, 119, e1819577.	0.8	17
3	Alkali metal doping of black phosphorus monolayer for ultrasensitive capture and detection of nitrogen dioxide. <i>Scientific Reports</i> , 2021, 11, 842.	1.6	9
4	Molecular-level insights into adsorption of a novel silyl ester donor on essential MgCl ₂ facets of supported Ziegler-Natta catalysts. <i>Journal of Physics and Chemistry of Solids</i> , 2021, 159, 110249.	1.9	3
5	Theoretical insights into sensing of hexavalent chromium on buckled and planar polymeric carbon nitride nanosheets of heptazine and triazine structures. <i>Molecular Simulation</i> , 2020, 46, 54-61.	0.9	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. <i>Adsorption</i> , 2020, 26, 429-442.	1.4	32
7	Influence of NiO decoration on adsorption capabilities of black phosphorus monolayer toward nitrogen dioxide: periodic DFT calculations. <i>Molecular Simulation</i> , 2020, 46, 1062-1072.	0.9	31
8	Defective phosphorene for highly efficient formaldehyde detection: Periodic density functional calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126792.	0.9	29
9	Highly improved carbon dioxide sensitivity and selectivity of black phosphorene sensor by vacancy doping: A quantum chemical perspective. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26265.	1.0	24
10	Defect engineering and zinc oxide doping of black phosphorene for nitrogen dioxide capture and detection: quantum-chemical calculations. <i>Applied Surface Science</i> , 2020, 523, 146527.	3.1	37
11	Hydrogen detection on black phosphorene doped with Ni, Pd, and Pt: Periodic density functional calculations. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 16298-16309.	3.8	35
12	Theoretical insights into hydrogen sensing capabilities of black phosphorene modified through ZnO doping and decoration. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 16918-16928.	3.8	35
13	Remarkable improvement in phosgene detection with a defect-engineered phosphorene sensor: first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9677-9684.	1.3	36
14	Mn-Doped black phosphorene for ultrasensitive hydrogen sulfide detection: periodic DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15549-15558.	1.3	26
15	Conductivity tuning of charged triazine and heptazine graphitic carbon nitride (g-C ₃ N ₄) quantum dots via nonmetal (B, O, S, P) doping: DFT calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2020, 141, 109422.	1.9	46
16	Quantum-chemical calculations on graphitic carbon nitride (g-C ₃ N ₄) single-layer nanostructures: polymeric slab vs. quantum dot. <i>Structural Chemistry</i> , 2020, 31, 1137-1148.	1.0	22
17	Phosphorene defects for high-quality detection of nitric oxide and carbon monoxide: A periodic density functional study. <i>Chemical Engineering Journal</i> , 2020, 396, 125247.	6.6	36
18	Substitutional doping of black phosphorene with boron, nitrogen, and arsenic for sulfur trioxide detection: a theoretical perspective. <i>Journal of Sulfur Chemistry</i> , 2020, 41, 399-420.	1.0	27

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19	Functionalization and Doping of Black Phosphorus. <i>Engineering Materials</i> , 2020, , 1-30.	0.3	11
20	Chemistry of Black Phosphorus. <i>Engineering Materials</i> , 2020, , 59-72.	0.3	12
21	Future Prospects and Challenges of Black Phosphorous Materials. <i>Engineering Materials</i> , 2020, , 157-169.	0.3	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. <i>Structural Chemistry</i> , 2019, 30, 85-96.	1.0	31
24	Kinetics of different bioreactor systems with <i>Acidithiobacillus ferrooxidans</i> for ferrous iron oxidation. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2019, 128, 611-627.	0.8	4
25	Superhydrophobic nanocomposite coatings of poly(methyl methacrylate) and stearic acid grafted CuO nanoparticles with photocatalytic activity. <i>Progress in Organic Coatings</i> , 2019, 136, 105270.	1.9	31
26	Synergistic Coconversion of Refinery Fuel Oil and Methanol over H-ZSM-5 Catalyst for Enhanced Production of Light Olefins. <i>Energy & Fuels</i> , 2019, 33, 5761-5765.	2.5	19
27	Dual role of ferric chloride in modification of USY catalyst for enhanced olefin production from refinery fuel oil. <i>Applied Catalysis A: General</i> , 2019, 580, 131-139.	2.2	10
28	Two-stage thermocatalytic upgrading of fuel oil to olefins and fuels over a nanoporous hierarchical acidic catalyst. <i>Petroleum Science and Technology</i> , 2019, 37, 1910-1916.	0.7	6
29	Structural diversity of metallacycle intermediates for ethylene dimerization on heterogeneous NiMCM-41 catalyst: a quantum chemical perspective. <i>Structural Chemistry</i> , 2019, 30, 137-150.	1.0	36
30	Steam catalytic cracking of fuel oil over a novel composite nanocatalyst: Characterization, kinetics and comparative perspective. <i>Journal of Analytical and Applied Pyrolysis</i> , 2019, 138, 281-293.	2.6	20
31	Molecular-level insights into furfural hydrogenation intermediates over single-atomic Cu catalysts on magnesia and silica nanoclusters. <i>Molecular Simulation</i> , 2019, 45, 154-163.	0.9	30
32	Catalytic transformation of ethylene to propylene and butene over an acidic Ca-incorporated composite nanocatalyst. <i>Applied Catalysis A: General</i> , 2019, 569, 20-27.	2.2	11
33	Thorough assessment of delayed coking correlations against literature data: Development of improved alternative models. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2019, 126, 83-102.	0.8	9
34	Combined effect of nanoporous diluent and steam on catalytic upgrading of fuel oil to olefins and fuels over USY catalyst. <i>Petroleum Science and Technology</i> , 2018, 36, 750-755.	0.7	21
35	Methane adsorption and hydrogen atom abstraction at diatomic radical cation metal oxo clusters: first-principles calculations. <i>Molecular Simulation</i> , 2018, 44, 850-863.	0.9	18
36	Influence of catalyst additives on vapor-phase hydrogenation of furfural to furfuryl alcohol on impregnated copper/magnesia. <i>Biomass Conversion and Biorefinery</i> , 2018, 8, 79-86.	2.9	20

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37	Heterogeneous catalysts for gas-phase conversion of ethylene to higher olefins. <i>Reviews in Chemical Engineering</i> , 2018, 34, 595-655.	2.3	50
38	HYDROTALCITE-IMPREGNATED COPPER AND CHROMIUM-DOPED COPPER AS NOVEL AND EFFICIENT CATALYSTS FOR VAPOR-PHASE HYDROGENATION OF FURFURAL: EFFECT OF CLAY PRETREATMENT. <i>Brazilian Journal of Chemical Engineering</i> , 2018, 35, 669-678.	0.7	11
39	Ethene Protonation Over Silica-Grafted Metal (Cr, Mo, and W) Oxide Catalysts: A Comparative Nanocluster Modeling Study. <i>Russian Journal of Inorganic Chemistry</i> , 2018, 63, 1570-1577.	0.3	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. <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2018, 54, 909-916.	0.3	16
41	Initiation of heterogeneous Schrock-type Mo and W oxide metathesis catalysts: A quantum thermochemical study. <i>Computational Materials Science</i> , 2018, 155, 197-208.	1.4	31
42	Nanostructured Hydrotalcite-Supported RuBaK Catalyst for Direct Conversion of Ethylene to Propylene. <i>Russian Journal of Applied Chemistry</i> , 2018, 91, 972-976.	0.1	13
43	Two-Step Thermal Cracking of an Extra-Heavy Fuel Oil: Experimental Evaluation, Characterization, and Kinetics. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 7421-7430.	1.8	41
44	A Novel Consecutive Approach for the Preparation of Cu-MgO Catalysts with High Activity for Hydrogenation of Furfural to Furfuryl Alcohol. <i>Catalysis Letters</i> , 2017, 147, 318-327.	1.4	40
45	Preparation of Cu-MgO catalysts with different copper precursors and precipitating agents for the vapor-phase hydrogenation of furfural. <i>Korean Journal of Chemical Engineering</i> , 2017, 34, 692-700.	1.2	24
46	Effect of promoter on selective hydrogenation of furfural over Cu-Cr/TiO ₂ catalyst. <i>Russian Journal of Applied Chemistry</i> , 2017, 90, 304-309.	0.1	9
47	Kinetic models for hydroconversion of furfural over the ecofriendly Cu-MgO catalyst: An experimental and theoretical study. <i>Applied Catalysis A: General</i> , 2017, 545, 134-147.	2.2	55
48	Comment on "hydrogen/methanol production in a novel multifunctional reactor with in situ adsorption: modeling and optimization". <i>International Journal of Energy Research</i> , 2017, 41, 461-462.	2.2	0
49	Cluster modeling and coordination structures of Cu ⁺ ions in Al-incorporated Cu-MEL catalysts: a density functional theory study. <i>Journal of the Mexican Chemical Society</i> , 2017, 61, .	0.2	28
50	Diversity of monomeric dioxo chromium species in Cr/silicalite-2 catalysts: A hybrid density functional study. <i>Computational Materials Science</i> , 2016, 118, 147-154.	1.4	25
51	Theoretical identification of structural heterogeneities of divalent nickel active sites in NiMCM-41 nanoporous catalysts. <i>Journal of Nanostructure in Chemistry</i> , 2016, 6, 365-372.	5.3	21
52	Characterization of extraframework Zn ²⁺ cationic sites in silicalite-2: a computational study. <i>Structural Chemistry</i> , 2016, 27, 467-475.	1.0	26
53	Removal of Cr(VI) Species from Aqueous Solution by Different Nanoporous Materials. <i>Iranian Journal of Toxicology</i> , 2016, 10, 15-21.	0.1	15
54	Saturated Five-membered N-Heterocyclic Carbene: A Computational Study. <i>Chemistry Letters</i> , 2015, 44, 1586-1588.	0.7	3

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55	Predictive correlations for thermal upgrading of petroleum residues. <i>Journal of Analytical and Applied Pyrolysis</i> , 2015, 115, 326-336.	2.6	22
56	Saturated N,X-Heterocyclic Carbenes (X=N, O, S, P, Si, C, and B): Stability, Nucleophilicity, and Basicity. <i>Australian Journal of Chemistry</i> , 2015, 68, 1438.	0.5	24
57	Comparison of four nanoporous catalysts in thermocatalytic upgrading of vacuum residue. <i>Journal of Analytical and Applied Pyrolysis</i> , 2013, 102, 97-102.	2.6	18
58	Applicability of protolytic mechanism to steady-state heterogeneous dehydrogenation of ethane revisited. <i>Microporous and Mesoporous Materials</i> , 2013, 170, 318-330.	2.2	21
59	Investigation of kinetics and cracked oil structural changes in thermal cracking of Iranian vacuum residues. <i>Fuel Processing Technology</i> , 2011, 92, 2226-2234.	3.7	49
60	Multivariable optimization of thermal cracking severity. <i>Chemical Engineering Research and Design</i> , 2011, 89, 1067-1077.	2.7	25
61	Evolutionary model for computation of pore-size distribution in microporous solids of cylindrical pore structure. <i>Microporous and Mesoporous Materials</i> , 2011, 138, 22-31.	2.2	10
62	Effect of Solvent Dearomatization and Operating Conditions in Steam Pyrolysis of a Heavy Feedstock. <i>Energy & Fuels</i> , 2010, 24, 1899-1907.	2.5	11
63	Flowsheeting of steam cracking furnaces. <i>Chemical Engineering Research and Design</i> , 2009, 87, 36-46.	2.7	46