Michael Badawi

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

143 papers	1,882 citations	25 h-index	35 g-index
155 ext. papers	2,570 ext. citations	5.2 avg, IF	5.56 L-index

#	Paper	IF	Citations
143	Molecular picture of the adsorption of phenol, toluene, carbon dioxide and water on kaolinite basal surfaces. *Applied Surface Science*, **2022**, 585, 152699	6.7	1
142	Stacking effect on electronic properties of InSe/blue phosphorene and GaSe/blue phosphorene heterostructures from first-principles. *Physica E: Low-Dimensional Systems and Nanostructures*, **2022**, 139, 115115	3	
141	Functionalized hydrochar-based catalysts for biodiesel production via oil transesterification: Optimum preparation conditions and performance assessment. *Fuel*, **2022**, 312, 122731	7.1	1
140	Polysaccharides in fabrication of membranes: A review.. *Carbohydrate Polymers*, **2022**, 281, 119041	10.3	12
139	Effect of Al3+ and Mg2+ on the flotation of fluorapatite using fatty- and hydroxamic-acid collectors □A multiscale investigation. *Applied Surface Science*, **2022**, 572, 151499	6.7	5
138	Impact of Sn doping on the hydrogen detection characteristics of ZnO thin films: Insights from experimental and DFT combination. *Applied Surface Science*, **2022**, 574, 151585	6.7	0
137	Performance and interactions of diclofenac adsorption using Alginate/Carbon-based Films: Experimental investigation and statistical physics modelling. *Chemical Engineering Journal*, **2022**, 428, 131929	14.7	9
136	High-Pressure Properties of Wolframite-Type ScNbO4. *Journal of Physical Chemistry C*, **2022**, 126, 4664-4676	3.7	2
135	Sustainable Downstream Separation of Itaconic Acid Using Carbon-Based Adsorbents. *Adsorption Science and Technology*, **2022**, 2022, 1-14	3.6	
134	Understanding the Cu adsorption mechanism on activated carbon using advanced statistical physics modelling.. *Environmental Science and Pollution Research*, **2022**, 1	5.1	
133	First-Principles Modeling of Dye Anchoring on (001) □Monoclinic WO3 Surfaces: The Role of Oxygen Vacancies. *Journal of Physical Chemistry C*, **2022**, 126, 5424-5434	3.8	1
132	Thermodynamics and Mechanism of the Adsorption of Heavy Metal Ions on Keratin Biomasses for Wastewater Detoxification. *Adsorption Science and Technology*, **2022**, 2022, 1-13	3.6	1
131	Layer-by-layer polymer deposited fabrics with superior flame retardancy and electrical conductivity. *Reactive and Functional Polymers*, **2022**, 173, 105221	4.6	0
130	Growth and annealing effect on the Cu thin film deposited on Si (0 0 1) surface. *Journal of Crystal Growth*, **2022**, 586, 126631	1.6	0
129	Ordered sodium zeolite-templated carbon with high first discharge capacity for sodium battery application. *Microporous and Mesoporous Materials*, **2022**, 336, 111853	5.3	2
128	Outstanding Performance of a New Exfoliated Clay Impregnated with Rutile TiO2 Nanoparticles Composite for Dyes Adsorption: Experimental and Theoretical Studies. *Coatings*, **2022**, 12, 22	2.9	1
127	Adaptation of advanced physical models to interpret the adsorption isotherms of lead and cadmium ions onto activated carbon in single-compound and binary systems.. *Environmental Science and Pollution Research*, **2022**, 1	5.1	

126	Synergistic effects between fatty acids and non-ionic reagents for the selective flotation of scheelite from a complex tungsten skarn ore. *Minerals Engineering*, **2022**, 182, 107566	4.9	1
125	Access to sodalite cages in ion-exchanged nanosized FAU zeolites probed by hyperpolarized 129Xe NMR and DFT calculations. *Microporous and Mesoporous Materials*, **2022**, 338, 111965	5.3	0
124	Enhanced adsorption of ketoprofen and 2,4-dichlorophenoxyactic acid on Physalis peruviana fruit residue functionalized with H2SO4: Adsorption properties and statistical physics modeling. *Chemical Engineering Journal*, **2022**, 445, 136773	14.7	0
123	Dynamics of Topology-dependent Water Purification by Siliceous Zeolite Membranes. *Journal of Molecular Liquids*, **2022**, 359, 119250	6	0
122	Insights Into the Mn(VII) and Cr(VI) Adsorption Mechanisms on Purified Diatomite/MCM-41 Composite: Experimental Study and Statistical Physics Analysis.. *Frontiers in Chemistry*, **2021**, 9, 814431	5	0
121	Engineered biochar: A way forward to environmental remediation. *Fuel*, **2021**, 122510	7.1	1
120	Graphene/g-carbon nitride (GO/g-CN) nanohybrids as a sensor material for the detection of methyl parathion and carbendazim.. *Chemosphere*, **2021**, 292, 133450	8.4	5
119	Low-dimensional HfS as SO adsorbent and gas sensor: effect of water and sulfur vacancies. *Physical Chemistry Chemical Physics*, **2021**, 23, 23655-23666	3.6	0
118	Co-precipitation polymerization of dual functional monomers and polystyrene--divinylbenzene for ciprofloxacin imprinted polymer preparation.. *RSC Advances*, **2021**, 11, 34281-34290	3.7	0
117	Hydration of magnesite and dolomite minerals: new insights from ab initio molecular dynamics. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2021**, 631, 127697	5.1	2
116	Beneficial effect of Au and Pt doping of the Ag-(100) surface for thiophene and pyridine adsorption from density functional theory calculations. *Chemical Physics*, **2021**, 553, 111391	2.3	0
115	Understanding the Pressure Effect on the Elastic, Electronic, Vibrational, and Bonding Properties of the CeScO3 Perovskite. *Journal of Physical Chemistry C*, **2021**, 125, 107-119	3.8	7
114	Theoretical study and analysis of o-nitrophenol adsorption using layered double hydroxides containing Ca-Al, Ni-Al and Zn-Al. *Environmental Science and Pollution Research*, **2021**, 28, 44547-44556	5.1	4
113	Interaction between fine particles of fluorapatite and phosphoric acid unraveled by surface spectroscopies. *Powder Technology*, **2021**, 382, 368-377	5.2	1
112	Hydration mechanisms of scheelite from adsorption isotherms and ab initio molecular dynamics simulations. *Applied Surface Science*, **2021**, 150137	6.7	8
111	Hybrid localized graph kernel for machine learning energy-related properties of molecules and solids. *Journal of Computational Chemistry*, **2021**, 42, 1390-1401	3.5	1
110	Make it clean, make it safe: A review on virus elimination via adsorption. *Chemical Engineering Journal*, **2021**, 412, 128682	14.7	9
109	Investigation of tautomerism of 1,3,5-triazine derivative, stability, and acidity of its tautomers from density functional theory. *Journal of Molecular Modeling*, **2021**, 27, 147	2	2

108	Single and simultaneous adsorption of Cr(VI) and Cu (II) on a novel Fe3O4/pine cones gel beads nanocomposite: Experiments, characterization and isotherms modeling. *Chemical Engineering Journal*, **2021**, 416, 129101	14.7	25
107	Understanding the Fundamentals of Microporosity Upgrading in Zeolites: Increasing Diffusion and Catalytic Performances. *Advanced Science*, **2021**, 8, e2100001	13.6	7
106	Elimination of Thiophenic Compounds by Cycloaddition with Ethylene for an Efficient Purification of Fuels: A DFT Study. *Topics in Catalysis*, **2021**, 64, 288-296	2.3	0
105	Simultaneous adsorption of acetaminophen, diclofenac and tetracycline by organo-sepiolite: Experiments and statistical physics modelling. *Chemical Engineering Journal*, **2021**, 404, 126601	14.7	28
104	An ab initio study of the electronic properties of the ferroelectric heterostructure In2Se3/Bi2Se3. *Applied Surface Science*, **2021**, 538, 148066	6.7	8
103	Molecular insights on the adsorption of some pharmaceutical residues from wastewater on kaolinite surfaces. *Chemical Engineering Journal*, **2021**, 407, 127176	14.7	21
102	Trapping of Ag+, Cu2+, and Co2+ by faujasite zeolite Y: New interpretations of the adsorption mechanism via DFT and statistical modeling investigation. *Chemical Engineering Journal*, **2021**, 420, 127712	14.7	13
101	Correlation Between Structure and Mechanical Properties of Amorphous Cu□Ag Alloys. *Physica Status Solidi (B): Basic Research*, **2021**, 258, 2000262	1.3	
100	Ab initio screening of zeolite Y formulations for efficient adsorption of thiophene in presence of benzene. *Applied Surface Science*, **2021**, 541, 148515	6.7	8
99	Sintering and deposition of homo- and heteronanoparticles of aluminum and nickel on aluminum (100) substrate. *Chemical Physics*, **2021**, 541, 111037	2.3	3
98	Effect of halogenation on the optical and electronic properties of tetrathienoanthracene and tetrathionoacridine derivatives: A DFT study. *Computational Condensed Matter*, **2021**, 26, e00528	1.7	
97	Adsorption mechanisms of fatty acids on fluorite unraveled by infrared spectroscopy and first-principles calculations. *Journal of Colloid and Interface Science*, **2021**, 583, 692-703	9.3	29
96	Adsorption of water in Na-LTA zeolites: an ab initio molecular dynamics investigation. *Physical Chemistry Chemical Physics*, **2021**, 23, 19032-19042	3.6	2
95	Adsorption of 3-aminophenol and resorcinol on avocado seed activated carbon: Mathematical modelling, thermodynamic study and description of adsorbent performance. *Journal of Molecular Liquids*, **2021**, 342, 116952	6	4
94	Adsorption of ketoprofen and 2- nitrophenol on activated carbon prepared from winery wastes: A combined experimental and theoretical study. *Journal of Molecular Liquids*, **2021**, 333, 115906	6	12
93	investigations of some compounds as potential anti-inflammatory inhibitors of 5-LO and LTA4H enzymes. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-16	3.6	1
92	Understanding the optical and bonding properties of hybrid metal-halide (C5H16NP) PbX4 (X□=□Cl, Br, I) perovskite: A density-functional theory study. *Inorganic Chemistry Communication*, **2021**, 130, 108721	3.1	1
91	Adsorption of Toluene and Water over Cationic-Exchanged Y Zeolites: A DFT Exploration. *Molecules* , **2021**, 26,	4.8	2

90	Nucleic Acids under Stress: Understanding and Simulating Nucleobase Fragmentation Pathways. *ChemPlusChem*, **2021**, 86, 1426-1435	2.8	
89	Ab initio investigation of the adsorption of phenolic compounds, CO, and H2O over metallic cluster/silica catalysts for hydrodeoxygenation process. *Applied Surface Science*, **2021**, 567, 150790	6.7	4
88	Selective adsorption of glucose towards itaconic acid on amorphous silica surfaces: Insights from density functional theory calculations. *Journal of Molecular Liquids*, **2021**, 343, 117586	6	1
87	One-step fabrication of a new outstanding rutile TiO2 nanoparticles/anthracite adsorbent: Modeling and physicochemical interpretations for malachite green removal. *Chemical Engineering Journal*, **2021**, 426, 131890	14.7	7
86	Ternary adsorption of cobalt, nickel and methylene blue on a modified chitin: Phenomenological modeling and physical interpretation of the adsorption mechanism. *International Journal of Biological Macromolecules*, **2020**, 158, 595-604	7.9	23
85	Synergistic adsorption of Pb2+ and CrO42□on an engineered biochar highlighted by statistical physical modeling. *Journal of Molecular Liquids*, **2020**, 312, 113483	6	15
84	DNA Nucleobase under Ionizing Radiation: Unexpected Proton Transfer by Thymine Cation in Water Nanodroplets. *Chemistry - A European Journal*, **2020**, 26, 11340-11344	4.8	2
83	Grafting of iron on amorphous silica surfaces from ab initio calculations. *Journal of Chemical Physics*, **2020**, 152, 214706	3.9	10
82	Fabrication and characterization of a thin coated adsorbent for antibiotic and analgesic adsorption: Experimental investigation and statistical physical modelling. *Chemical Engineering Journal*, **2020**, 401, 126007	14.7	21
81	Origin of the outstanding performance of ZnAl and MgFe layered double hydroxides in the adsorption of 2-nitrophenol: A statistical physics assessment. *Journal of Molecular Liquids*, **2020**, 314, 113572	6	6
80	Copper-enriched diamond-like carbon coatings promote regeneration at the bone-implant interface. *Heliyon*, **2020**, 6, e03798	3.6	15
79	The Challenge of Tungsten Skarn Processing by Froth Flotation: A Review. *Frontiers in Chemistry*, **2020**, 8, 230	5	13
78	Effects of Wall Slip on Convective Heat Transfers of Giesekus Fluid in Microannulus. *Journal of Heat Transfer*, **2020**, 142,	1.8	1
77	Synergistic adsorption of lanthanum ions and fatty acids for efficient rare-earth phosphate recovery: Surface analysis and ab initio molecular dynamics studies. *Applied Surface Science*, **2020**, 526, 146725	6.7	13
76	Kinetic, thermodynamic and mechanism study of the adsorption of phenol on Moroccan clay. *Journal of Molecular Liquids*, **2020**, 312, 113383	6	24
75	Improved tribological properties, thermal and colloidal stability of poly-□blefins based lubricants with hydrophobic MoS submicron additives. *Journal of Colloid and Interface Science*, **2020**, 562, 91-101	9.3	13
74	Physicochemical interpretation of the adsorption of 4-Bromophenol and 4-Chloroaniline on an activated carbon. *Journal of Environmental Chemical Engineering*, **2020**, 8, 104542	6.8	8
73	Statistical physics interpretation of the adsorption mechanism of Pb2+, Cd2+ and Ni2+ on chicken feathers. *Journal of Molecular Liquids*, **2020**, 319, 114168	6	20

72	Adsorption of methylene blue on silica nanoparticles: Modelling analysis of the adsorption mechanism via a double layer model. *Journal of Molecular Liquids*, **2020**, 319, 114348	6	13
71	Structure, stability, and surface diffusion of clusters: Pt4/Cu (110) AND Au4/Ag (110) surface by molecular dynamics. *EPJ Applied Physics*, **2020**, 91, 31302	1.1	2
70	Biofuel purification: Coupling experimental and theoretical investigations for efficient separation of phenol from aromatics by zeolites. *Chemical Engineering Journal*, **2020**, 402, 126264	14.7	23
69	Understanding the adsorption mechanism of Ag+ and Hg2+ on functionalized layered double hydroxide via statistical physics modeling. *Applied Clay Science*, **2020**, 198, 105828	5.2	15
68	Interaction between transition metals (Co, Ni, and Cu) systems and amorphous silica surfaces: A DFT investigation. *Applied Surface Science*, **2020**, 533, 147422	6.7	11
67	Water-silanol interactions on the amorphous silica surface: A dispersion-corrected DFT investigation. *Journal of Molecular Liquids*, **2020**, 320, 114496	6	1
66	Disclosing the behavior under hydrostatic pressure of rhombohedral MgInSe by means of first-principles calculations. *Physical Chemistry Chemical Physics*, **2020**, 22, 21909-21918	3.6	3
65	Structure-Elasticity Relationship of Potassium Silicate Glasses from Brillouin Light Scattering Spectroscopy and Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2020**, 124, 9216-9223	3.4	2
64	drug discovery of IKK-□nhibitors from 2-amino-3-cyano-4-alkyl-6-(2-hydroxyphenyl) pyridine derivatives based on QSAR, docking, molecular dynamics and drug-likeness evaluation studies. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-17	3.6	8
63	Assessing the Potential of Amorphous Silica Surfaces for the Removal of Phenol from Biofuel: A Density Functional Theory Investigation. *Journal of Physical Chemistry C*, **2020**, 124, 20262-20269	3.8	8
62	Imprinting isolated single iron atoms onto mesoporous silica by templating with metallosurfactants. *Journal of Colloid and Interface Science*, **2020**, 573, 193-203	9.3	15
61	Incorporation of trivalent cations in NaX zeolite nanocrystals for the adsorption of O in the presence of CO. *Physical Chemistry Chemical Physics*, **2020**, 22, 9934-9942	3.6	6
60	Quantum Effects on the Diffusivity of Hydrogen Isotopes in Zeolites. *Journal of Physical Chemistry C* , **2019**, 123, 23455-23463	3.8	8
59	A review of atomistic simulation methods for surface physical-chemistry phenomena applied to froth flotation. *Minerals Engineering*, **2019**, 143, 106020	4.9	37
58	Relationship between electronic structures and antiplasmodial activities of xanthone derivatives: a 2D-QSAR approach. *Structural Chemistry*, **2019**, 30, 2301-2310	1.8	
57	A first principle evaluation of the adsorption mechanism and stability of volatile organic compounds into NaY zeolite. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2019**, 234, 469-482	1	17
56	An ab initio study of the ferroelectric In2Se3/graphene heterostructure. *Physica E: Low-Dimensional Systems and Nanostructures*, **2019**, 114, 113582	3	12
55	Computational insights into the structure of barium titanosilicate glasses. *Journal of the American Ceramic Society*, **2019**, 102, 6626-6639	3.8	8

54	Dibenzyl Disulfide Adsorption on Cationic Exchanged Faujasites: A DFT Study. *Nanomaterials*, **2019**, 9,	5.4	12
53	Pressure effects on local atomic structure of Ni15Co15Al70 metallic glasses. *Computational Materials Science*, **2019**, 166, 20-29	3.2	7
52	Ab initio screening of cation-exchanged zeolites for biofuel purification. *Molecular Systems Design and Engineering*, **2019**, 4, 882-892	4.6	25
51	Benchmarking the performance of approximate van der Waals methods for the structural and energetic properties of SiO and AlPO frameworks. *Journal of Chemical Physics*, **2019**, 150, 094102	3.9	14
50	Adsorption of volatile organic and iodine compounds over silver-exchanged mordenites: A comparative periodic DFT study for several silver loadings. *Applied Surface Science*, **2019**, 485, 56-63	6.7	30
49	Ionization and fragmentation of uracil upon microhydration. *Physical Chemistry Chemical Physics*, **2019**, 21, 4810-4821	3.6	10
48	Ab Initio Study of the Stepwise versus Concerted Fragmentation Pathways in Microhydrated Thymine Radical Cations. *Chemistry - A European Journal*, **2019**, 25, 15525-15534	4.8	3
47	Adsorption and diffusion of Pt, Cu, Ag and Au on missing row reconstructed Pt(110) surfaces: An ab initio investigation. *Surface Science*, **2019**, 690, 121463	1.8	3
46	Surface chemistry of halloysite nanotubes controls the curability of low filled epoxy nanocomposites. *Progress in Organic Coatings*, **2019**, 135, 555-564	4.8	46
45	Electronic structure and optical properties of isolated and TiO -grafted free base porphyrins for water oxidation: A challenging test case for DFT and TD-DFT. *Journal of Computational Chemistry*, **2019**, 40, 2530-2538	3.5	2
44	Quantum mechanistic study of furan and 2-methylfuran hydrodeoxygenation on molybdenum and tungsten sulfide clusters. *Journal of Molecular Modeling*, **2019**, 25, 237	2	4
43	Atomistic description of phenol, CO and H2O adsorption over crystalline and amorphous silica surfaces for hydrodeoxygenation applications. *Applied Surface Science*, **2019**, 494, 721-730	6.7	17
42	Untangling electronic, optical and bonding properties of hexagonal bismuth borate SrBi2B2O7 crystal for ultraviolet opto-electronic applications: An ab initio study. *Journal of Alloys and Compounds*, **2019**, 803, 1127-1135	5.7	6
41	Computing RPA Adsorption Enthalpies by Machine Learning Thermodynamic Perturbation Theory. *Journal of Chemical Theory and Computation*, **2019**, 15, 6333-6342	6.4	21
40	Bridging molecular dynamics and correlated wave-function methods for accurate finite-temperature properties. *Physical Review Materials*, **2019**, 3,	3.2	10
39	Comment on: Effects of crystal chemistry on sodium oleate adsorption on fluorite surface investigated by molecular dynamics simulation: Renji Zheng, Zijie Ren, Huimin Gao, Zhijie Chen, Yupeng Qian, Yubiao Li, Minerals Engineering, vol. 124, pp. 77-85, 2018. *Minerals Engineering*, **2019**, 135, 156-159	4.9	2
38	Synergistic adsorptions of NaCO and NaSiO on calcium minerals revealed by spectroscopic and molecular dynamics studies. *Chemical Science*, **2019**, 10, 9928-9940	9.4	22
37	Evaluation of the Inhibiting Effect of Organic Compounds on the Adsorption of Iodine Compounds in Cation-Exchanged Zeolites: A DFT Study. *Advances in Science, Technology and Innovation*, **2018**, 107-109	8.3	4

36	Surface Properties of Fluorite in Presence of Water: An Atomistic Investigation. *Journal of Physical Chemistry B*, **2018**, 122, 6829-6836	3.4	27
35	Elastic and structural properties of low silica calcium aluminosilicate glasses from molecular dynamics simulations. *Journal of Non-Crystalline Solids*, **2018**, 499, 142-152	3.9	8
34	New reagent formulations for selective flotation of scheelite from a skarn ore with complex calcium minerals gangue. *Minerals Engineering*, **2018**, 123, 85-94	4.9	44
33	Comparative study of structural and electronic properties of GaSe and InSe polytypes. *Journal of Chemical Physics*, **2018**, 149, 054106	3.9	23
32	Proton Mobility, Intrinsic Acid Strength, and Acid Site Location in Zeolites Revealed by Varying Temperature Infrared Spectroscopy and Density Functional Theory Studies. *Journal of the American Chemical Society*, **2018**, 140, 17790-17799	16.4	31
31	Molecular Insight into Fatty Acid Adsorption on Bare and Hydrated (111) Fluorite Surface. *Journal of Physical Chemistry B*, **2018**, 122, 12403-12410	3.4	35
30	Adsorption of NO, NO2, CO, H2O and CO2 over isolated monovalent cations in faujasite zeolite: a periodic DFT investigation. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	27
29	Selective Capture of Phenol from Biofuel Using Protonated Faujasite Zeolites with Different Si/Al Ratios. *Journal of Physical Chemistry C*, **2018**, 122, 26419-26429	3.8	32
28	A DFT study of RuO interactions with porous materials: metal-organic frameworks (MOFs) and zeolites. *Physical Chemistry Chemical Physics*, **2018**, 20, 16770-16776	3.6	19
27	Forced convection heat transfer of Giesekus fluid with wall slip above the critical shear stress in pipes. *International Journal of Heat and Fluid Flow*, **2018**, 71, 442-450	2.4	3
26	Curing behavior of epoxy/Fe3O4 nanocomposites: A comparison between the effects of bare Fe3O4, Fe3O4/SiO2/chitosan and Fe3O4/SiO2/chitosan/imide/phenylalanine-modified nanofillers. *Progress in Organic Coatings*, **2018**, 123, 10-19	4.8	78
25	Competing structures in (In,Ga)Se and (In,Ga)2Se3 semiconductors. *Physica Status Solidi (B): Basic Research*, **2017**, 254, 1700120	1.3	5
24	Performance of Cu -, Pb -, and Hg -Exchanged Mordenite in the Adsorption of I , ICH , H O, CO, ClCH , and Cl : A Density Functional Study. *ChemPhysChem*, **2017**, 18, 1642-1652	3.2	19
23	Dissociative iodomethane adsorption on Ag-MOR and the formation of AgI clusters: an ab initio molecular dynamics study. *Physical Chemistry Chemical Physics*, **2017**, 19, 27530-27543	3.6	29
22	Influence of water, dihydrogen and dioxygen on the stability of the Cr2O3 surface: A first-principles investigation. *Surface Science*, **2017**, 666, 44-52	1.8	11
21	Thermodynamic and structural properties of binary calcium silicate glasses: insights from molecular dynamics. *Physical Chemistry Chemical Physics*, **2017**, 19, 19083-19093	3.6	17
20	Syntheses, crystal structures, and optical properties of CsBa5Ti2Se9Cl and CsBa2Cl5. *Journal of Solid State Chemistry*, **2017**, 253, 258-262	3.3	2
19	Evaluation of volatile iodine trapping in presence of contaminants: A periodic DFT study on cation exchanged-faujasite. *Microporous and Mesoporous Materials*, **2017**, 239, 111-122	5.3	36

18	Impact of the Si/Al ratio on the selective capture of iodine compounds in silver-mordenite: a periodic DFT study. *Physical Chemistry Chemical Physics*, **2016**, 18, 25574-25581	3.6	28
17	Crystal structure and energy bands of (Ga/In)Se and Cu(In,Ga)Se2 semiconductors in comparison. *Physica Status Solidi (B): Basic Research*, **2016**, 253, 1472-1475	1.3	13
16	Effect of Sodium Oxide Modifier on Structural and Elastic Properties of Silicate Glass. *Journal of Physical Chemistry B*, **2016**, 120, 13193-13205	3.4	45
15	A DFT investigation of the adsorption of iodine compounds and water in H-, Na-, Ag-, and Cu-mordenite. *Journal of Chemical Physics*, **2016**, 144, 244705	3.9	45
14	A DFT study of the hematite surface state in the presence of H2, H2O and O2. *Surface Science*, **2013**, 610, 7-15	1.8	36
13	Hydrodeoxygenation of Phenolic Compounds by Sulfided (Co)Mo/Al2O3Catalysts, a Combined Experimental and Theoretical Study. *Oil and Gas Science and Technology*, **2013**, 68, 829-840	1.9	32
12	Molecular structures and thermodynamic properties of 12 gaseous cesium-containing species of nuclear safety interest: Cs2, CsH, CsO, Cs2O, CsX, and Cs2X2 (X = OH, Cl, Br, and I). *Journal of Nuclear Materials*, **2012**, 420, 452-462	3.3	25
11	Ab initio calculations and iodine kinetic modeling in the reactor coolant system of a pressurized water reactor in case of severe nuclear accident. *Computational and Theoretical Chemistry*, **2012**, 990, 194-208	2	21
10	n-Heptane cracking over mixtures of HY and HZSM-5 zeolites: Influence of the presence of phenol. *Fuel*, **2012**, 94, 571-577	7.1	19
9	Guaiacol derivatives and inhibiting species adsorption over MoS2 and CoMoS catalysts under HDO conditions: A DFT study. *Catalysis Communications*, **2011**, 12, 901-905	3.2	65
8	Effect of water on the stability of Mo and CoMo hydrodeoxygenation catalysts: A combined experimental and DFT study. *Journal of Catalysis*, **2011**, 282, 155-164	7.3	135
7	Kinetic study of olefin hydrogenation on hydrotreating catalysts. *Journal of Molecular Catalysis A*, **2010**, 320, 34-39		24
6	DFT study of furan adsorption over stable molybdenum sulfide catalyst under HDO conditions. *Comptes Rendus Chimie*, **2009**, 12, 754-761	2.7	43
5	Promoting effect of cobalt and nickel on the activity of hydrotreating catalysts in hydrogenation and isomerization of olefins. *Journal of Molecular Catalysis A*, **2008**, 293, 53-58		35
4	Contribution of DFT to the optimization of Ni-based catalysts for dry reforming of methane: a review. *Catalysis Reviews - Science and Engineering*,1-53	12.6	1
3	Latex/AgNPs: Synthesis, and Their Antibacterial Activity. *Journal of Cluster Science*,1	3	0
2	Competitive adsorption of phenol and toluene onto silica-supported transition metal clusters for biofuel purification. *Molecular Systems Design and Engineering*,	4.6	3
1	Elucidation of the IR of Cu and Mn substituted intraframework SiBEA zeolites. *Topics in Catalysis*,1	2.3	