

# Mohammednoor K Altarawneh

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3751626/publications.pdf>

Version: 2024-02-01

219  
papers

4,401  
citations

147786  
31  
h-index

182417  
51  
g-index

220  
all docs

220  
docs citations

220  
times ranked

3870  
citing authors

#	ARTICLE	IF	CITATIONS
1	Molybdenum nitrides from structures to industrial applications. <i>Reviews in Chemical Engineering</i> , 2023, 39, 329-361.	4.4	7
2	Torrefaction of Densified Woody Biomass: The Effect of Pellet Size on Thermochemical and Thermophysical Characteristics. <i>Bioenergy Research</i> , 2022, 15, 544-558.	3.9	7
3	Thermal decomposition of perfluorinated carboxylic acids: Kinetic model and theoretical requirements for PFAS incineration. <i>Chemosphere</i> , 2022, 286, 131685.	8.2	48
4	Temperature-dependent profiles of dioxin-like toxicants from combustion of brominated flame retardants. <i>Journal of Hazardous Materials</i> , 2022, 422, 126879.	12.4	17
5	CO2 capture and ions removal through reaction with potassium hydroxide in desalination reject brine: Statistical optimization. <i>Chemical Engineering and Processing: Process Intensification</i> , 2022, 170, 108722.	3.6	13
6	Removal of Bromine from the non-metallic fraction in printed circuit board via its Co-pyrolysis with alumina. <i>Waste Management</i> , 2022, 137, 283-293.	7.4	31
7	Thermal decomposition of heptafluoropropylene-oxide-dimer acid (GenX). <i>Chemosphere</i> , 2022, 289, 133118.	8.2	8
8	Catalytic upgrading of the polymeric constituents in Covid-19 masks. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 106978.	6.7	23
9	On the formation chemistry of brominated polycyclic aromatic hydrocarbons (BrPAHs). <i>Chemosphere</i> , 2022, 290, 133367.	8.2	5
10	Bromination mechanisms of aromatic pollutants: formation of Br2 and bromine transfer from metallic oxybromides. <i>Environmental Science and Pollution Research</i> , 2022, , 1.	5.3	2
11	Ceria-supported niobium oxide catalyst for low-temperature oxidation of 1,3-butadiene. <i>Molecular Catalysis</i> , 2022, 518, 112083.	2.0	1
12	Computational Insights in DNA Methylation: Catalytic and Mechanistic Elucidations for Forming 3-Methyl Cytosine. <i>Journal of Chemistry</i> , 2022, 2022, 1-11.	1.9	1
13	Selective Hydrogenation of 1,3-Butadiene over Ceria Catalyst: A Molecular Insight. <i>Molecular Catalysis</i> , 2022, 524, 112331.	2.0	3
14	Exploring the potential of hematite as a debromination agent for 2,4,6-tribromophenol. <i>Chemical Engineering Journal Advances</i> , 2022, 11, 100334.	5.2	10
15	Thermodynamic stability of niobium-doped ceria surfaces. <i>Journal of Molecular Structure</i> , 2022, 1265, 133416.	3.6	2
16	Probing the chemical reactivity of the B2O3 -I (1 0 1) Surface: Interaction with H2O and H2S. <i>Applied Surface Science</i> , 2022, 599, 153999.	6.1	0
17	Kinetics of antigorite dehydroxylation for CO2 sequestration. <i>Minerals Engineering</i> , 2022, 184, 107630.	4.3	2
18	Thermal decomposition of ammonium nitrate on rust surface: Risk of low-temperature fire. <i>Fire Safety Journal</i> , 2021, 120, 103063.	3.1	9

#	ARTICLE	IF	CITATIONS
19	Flammability of sulfur powder - An extremely hazardous chemical. <i>Fire Safety Journal</i> , 2021, 120, 103088.	3.1	0
20	Combustion chemistry of COS and occurrence of intersystem crossing. <i>Fuel</i> , 2021, 283, 119257.	6.4	15
21	Toxicology and environmental chemistry of halogenated organic pollutants. <i>Ecotoxicology and Environmental Safety</i> , 2021, 207, 111573.	6.0	2
22	Review of Chemical Reactivity of Singlet Oxygen with Organic Fuels and Contaminants. <i>Chemical Record</i> , 2021, 21, 315-342.	5.8	59
23	A chemical kinetic model for the decomposition of perfluorinated sulfonic acids. <i>Chemosphere</i> , 2021, 263, 128256.	8.2	24
24	Atmospheric chemistry of oxazole: the mechanism and kinetic studies of the oxidation reaction initiated by OH radicals. <i>New Journal of Chemistry</i> , 2021, 45, 2237-2248.	2.8	15
25	Ceria-Based Catalysts for Selective Hydrogenation Reactions: A Critical Review. <i>Catalysis Surveys From Asia</i> , 2021, 25, 27-47.	2.6	19
26	A kinetic model for halogenation of the zinc content in franklinite. <i>Applied Surface Science</i> , 2021, 562, 150105.	6.1	13
27	Exploring reactions of amines-model compounds with NH <sub>2</sub> : In relevance to nitrogen conversion chemistry in biomass. <i>Fuel</i> , 2021, 291, 120076.	6.4	12
28	Effects of potassium hydroxide and aluminum oxide on the performance of a modified solvay process for CO <sub>2</sub> capture: A comparative study. <i>International Journal of Energy Research</i> , 2021, 45, 13952-13964.	4.5	22
29	Controlling NO <sub>x</sub> emission from boilers using waste polyethylene as reburning fuel. <i>Chemical Engineering Journal</i> , 2021, 411, 128427.	12.7	16
30	Updated yields of nitrogenated species in flames of ammonia/benzene via introducing an aniline sub-mechanism. <i>Combustion and Flame</i> , 2021, 228, 433-442.	5.2	7
31	High temperature (up to 1200°C) thermal-mechanical stability of Si and Ni doped CrN framework coatings. <i>Journal of Materials Research and Technology</i> , 2021, 14, 2406-2419.	5.8	5
32	KOH-Based Modified Solvay Process for Removing Na Ions from High Salinity Reject Brine at High Temperatures. <i>Sustainability</i> , 2021, 13, 10200.	3.2	15
33	Mineralisation of atmospheric CO <sub>2</sub> in hydromagnesite in ultramafic mine tailings – Insights from Mg isotopes. <i>Geochimica Et Cosmochimica Acta</i> , 2021, 309, 191-208.	3.9	10
34	Low-temperature oxidation of monobromobenzene: Bromine transformation and yields of phenolic species. <i>Chemosphere</i> , 2021, 280, 130621.	8.2	8
35	Very-few-layer graphene obtained from facile two-step shear exfoliation in aqueous solution. <i>Chemical Engineering Science</i> , 2021, 245, 116848.	3.8	10
36	Nanosystem's density functional theory study of the chlorine adsorption on the Fe(100) surface. <i>Nanotechnology Reviews</i> , 2021, 10, 719-727.	5.8	5

#	ARTICLE	IF	CITATIONS
37	An Insight into Geometries and Catalytic Applications of CeO <sub>2</sub> from a DFT Outlook. <i>Molecules</i> , 2021, 26, 6485.	3.8	14
38	A closer look into the contribution of atmospheric gas-phase pathways in the formation of perfluorocarboxylic acids. <i>Atmospheric Pollution Research</i> , 2021, 12, 101255.	3.8	8
39	Leaching behavior of zinc and lead from electric arc furnace dust " Poly(vinyl) chloride residues after oxidative thermal treatment. <i>Journal of Cleaner Production</i> , 2021, 328, 129622.	9.3	15
40	Investigative properties of CeO <sub>2</sub> doped with niobium: A combined characterization and DFT studies. <i>Nanotechnology Reviews</i> , 2021, 11, 191-203.	5.8	11
41	Formation of phenoxy-type Environmental Persistent Free Radicals (EPFRs) from dissociative adsorption of phenol on Cu/Fe and their partial oxides. <i>Chemosphere</i> , 2020, 240, 124921.	8.2	17
42	Influence of the variation in the Hubbard parameter ( $U$ ) on activation energies of CeO <sub>2</sub> -catalysed reactions. <i>Canadian Journal of Physics</i> , 2020, 98, 385-389.	1.1	7
43	Physico-chemical properties of CrMoN coatings - combined experimental and computational studies. <i>Thin Solid Films</i> , 2020, 693, 137671.	1.8	13
44	Burning properties of redox crystals of ammonium nitrate and saccharides. <i>Combustion and Flame</i> , 2020, 213, 132-139.	5.2	13
45	Analytical Procedure for Proximate Analysis of Algal Biomass: Case Study for <i>Spirulina platensis</i> and <i>Chlorella vulgaris</i> . <i>Energy &amp; Fuels</i> , 2020, 34, 474-482.	5.1	19
46	Adsorption and dissociation of the methanethiol (CH <sub>3</sub> SH) molecule on the Fe(100) surface. <i>Surface and Interface Analysis</i> , 2020, 52, 156-166.	1.8	5
47	Singlet-diradical character in large PAHs triggers spontaneous-ignition of coal. <i>Combustion and Flame</i> , 2020, 212, 279-281.	5.2	10
48	Interfacial and bulk properties of concentrated solutions of ammonium nitrate. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 27698-27712.	2.8	9
49	A computational study on the kinetics of pyrolysis of isopropyl propionate as a biodiesel model: DFT and ab initio investigation. <i>Fuel</i> , 2020, 281, 118798.	6.4	18
50	A kinetic model for evolution of H <sub>2</sub> and CO over Zr-doped ceria. <i>Molecular Catalysis</i> , 2020, 498, 111256.	2.0	3
51	Computational mechanistic study of the unimolecular dissociation of ethyl hydroperoxide and its bimolecular reactions with atmospheric species. <i>Scientific Reports</i> , 2020, 10, 15025.	3.3	2
52	Formation of polybrominated dibenzofurans (PBDFs) and polybrominated diphenyl ethers (PBDEs) from oxidation of brominated flame retardants (BFRs). <i>Journal of Hazardous Materials</i> , 2020, 400, 123166.	12.4	14
53	Co-pyrolysis of polyethylene with products from thermal decomposition of brominated flame retardants. <i>Chemosphere</i> , 2020, 254, 126766.	8.2	8
54	Photodecomposition properties of brominated flame retardants (BFRs). <i>Ecotoxicology and Environmental Safety</i> , 2020, 192, 110272.	6.0	15

#	ARTICLE	IF	CITATIONS
55	Computational Study of the Dissociation Reactions of Secondary Ozonide. <i>Atmosphere</i> , 2020, 11, 100.	2.3	4
56	Kinetics of Photo-Oxidation of Oxazole and its Substituents by Singlet Oxygen. <i>Scientific Reports</i> , 2020, 10, 3668.	3.3	7
57	Selective and sensitive visible-light-prompt photoelectrochemical sensor of Cu <sup>2+</sup> based on CdS nanorods modified with Au and graphene quantum dots. <i>Journal of Hazardous Materials</i> , 2020, 391, 122248.	12.4	29
58	Products of incomplete combustion from biomass reburning. <i>Fuel</i> , 2020, 274, 117805.	6.4	16
59	Importance of Intersystem Crossing on Flammability Properties of Carbon Disulphide (CS <sub>2</sub> )., 2020, , 77-88.		0
60	Effect of Fe <sub>2</sub> O <sub>3</sub> nanoparticles on combustion of coal surrogate (Anisole): Enhanced ignition and formation of persistent free radicals. <i>Proceedings of the Combustion Institute</i> , 2019, 37, 3091-3099.	3.9	18
61	Biocompatibility study of multi-layered hydroxyapatite coatings synthesized on Ti-6Al-4V alloys by RF magnetron sputtering for prosthetic-orthopaedic implant applications. <i>Applied Surface Science</i> , 2019, 463, 292-299.	6.1	42
62	Formation of polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/F) from oxidation of 4,4'-dichlorobiphenyl (4,4'-DCB). <i>Proceedings of the Combustion Institute</i> , 2019, 37, 1075-1082.	3.9	12
63	Probing the Reactivity of Singlet Oxygen with Cyclic Monoterpenes. <i>ACS Omega</i> , 2019, 4, 14040-14048.	3.5	7
64	Mg isotope fractionation during continental weathering and low temperature carbonation of ultramafic rocks. <i>Geochimica Et Cosmochimica Acta</i> , 2019, 262, 60-77.	3.9	24
65	Synthesis and Characterization of $\beta^2$ -Diketimine Schiff Base Complexes with Ni(II) and Zn(II) Ions: Experimental and Theoretical Study. <i>Journal of Chemistry</i> , 2019, 2019, 1-9.	1.9	1
66	Reaction of Hydroperoxy Radicals with Primary C <sub>5</sub> Alcohols: A Profound Effect on Ignition Delay Times. <i>Energy &amp; Fuels</i> , 2019, 33, 11781-11794.	5.1	16
67	Destruction of dioxin and furan pollutants via electrophilic attack of singlet oxygen. <i>Ecotoxicology and Environmental Safety</i> , 2019, 184, 109605.	6.0	15
68	A computational study of the ozonolysis of sabinene. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	1.4	11
69	Reaction of phenol with singlet oxygen. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 171-183.	2.8	75
70	A first-principles study of the electronic, structural, and optical properties of CrN and Mo:CrN clusters. <i>Ceramics International</i> , 2019, 45, 17094-17102.	4.8	4
71	The mechanism of electrophilic addition of singlet oxygen to pyrrolic ring. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	1.4	8
72	Thermal decomposition of model compound of algal biomass. <i>International Journal of Chemical Kinetics</i> , 2019, 51, 696-710.	1.6	7

#	ARTICLE	IF	CITATIONS
73	Hydrostatic bath synthesis of conductive polypyrrole/reduced graphene oxide aerogel as compression sensor. <i>European Polymer Journal</i> , 2019, 117, 227-235.	5.4	18
74	Catalytic de-chlorination of products from PVC degradation by magnetite (Fe <sub>3</sub> O <sub>4</sub> ). <i>Applied Surface Science</i> , 2019, 480, 792-801.	6.1	15
75	Nanorose-like ZnCo <sub>2</sub> O <sub>4</sub> coatings synthesized via sol-gel route: morphology, grain growth and DFT simulations. <i>Journal of Sol-Gel Science and Technology</i> , 2019, 90, 450-464.	2.4	3
76	Studies of annealing impact on the morphological, opto-dielectric and mechanical behaviors of molybdenum-doped CrN coatings. <i>Thin Solid Films</i> , 2019, 677, 119-129.	1.8	5
77	A Thermochemical Parameters and Theoretical Study of the Chlorinated Compounds of Thiophene. <i>Heteroatom Chemistry</i> , 2019, 2019, 1-6.	0.7	0
78	A holistic analysis of surface, chemical bonding states and mechanical properties of sol-gel synthesized CoZn-oxide coatings complemented by finite element modeling. <i>Ceramics International</i> , 2019, 45, 10882-10898.	4.8	5
79	Unimolecular Decomposition Reactions of Propylamine and Protonated Propylamine. <i>ACS Omega</i> , 2019, 4, 3306-3313.	3.5	15
80	Combustion chemistry of carbon disulphide (CS <sub>2</sub> ). <i>Combustion and Flame</i> , 2019, 210, 413-425.	5.2	16
81	Co-oxidation of methane (CH <sub>4</sub> ) and carbon disulfide (CS <sub>2</sub> ). <i>Proceedings of the Combustion Institute</i> , 2019, 37, 677-685.	3.9	8
82	Thermodynamic Analysis on the Oxidative Pyrolytic Treatment of Electric Arc Furnace Dust-TBBA Blends. <i>Oxidation of Metals</i> , 2019, 91, 561-588.	2.1	7
83	The gas-phase ozonolysis reaction of methylbutenol: A mechanistic study. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25888.	2.0	5
84	Interaction of NH <sub>2</sub> radical with alkylbenzenes. <i>Combustion and Flame</i> , 2019, 200, 85-96.	5.2	9
85	Thermal decomposition of brominated flame retardants (BFRs): Products and mechanisms. <i>Progress in Energy and Combustion Science</i> , 2019, 70, 212-259.	31.2	168
86	Hydration and Secondary Ozonide of the Criegee Intermediate of Sabinene. <i>ACS Omega</i> , 2018, 3, 2417-2427.	3.5	10
87	Pyrolysis kinetics of tetrabromobisphenol a (TBBPA) and electric arc furnace dust mixtures. <i>Thermochimica Acta</i> , 2018, 660, 61-69.	2.7	22
88	Thermo-mechanical properties of cubic lanthanide oxides. <i>Thin Solid Films</i> , 2018, 653, 37-48.	1.8	10
89	Understanding the impacts of Al <sup>3+</sup> -substitutions on the enhancement of magnetic, dielectric and electrical behaviors of ceramic processed nickel-zinc mixed ferrites: FTIR assisted studies. <i>Materials Research Bulletin</i> , 2018, 97, 444-451.	5.2	22
90	Recycling of zincite (ZnO) via uptake of hydrogen halides. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1221-1230.	2.8	26

#	ARTICLE	IF	CITATIONS
91	The ozonolysis of cyclic monoterpenes: a computational review. Canadian Journal of Chemistry, 2018, 96, 281-292.	1.1	13
92	Thermo-mechanical properties of cubic titanium nitride. Molecular Simulation, 2018, 44, 415-423.	2.0	11
93	Thermal Analysis on the Pyrolysis of Tetrabromobisphenol A and Electric Arc Furnace Dust Mixtures. Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science, 2018, 49, 45-60.	2.1	17
94	Thermochemical parameters of chlorinated compounds of pyridine. Computational and Theoretical Chemistry, 2018, 1146, 21-26.	2.5	1
95	Catalytic de-halogenation of alkyl halides by copper surfaces. Journal of Environmental Chemical Engineering, 2018, 6, 7214-7224.	6.7	5
96	Development of Organo-Dispersible Graphene Oxide via Pseudo-Surface Modification for Thermally Conductive Green Polymer Composites. ACS Omega, 2018, 3, 18124-18131.	3.5	8
97	Catalytic Hydrogenation of <i>p</i> -Chloronitrobenzene to <i>p</i> -Chloroaniline Mediated by $\text{I}^{\text{III}}\text{-Mo}_2\text{N}$ . ACS Omega, 2018, 3, 14380-14391.	3.5	15
98	Role of Singlet Oxygen in Combustion Initiation of Aromatic Fuels. Energy & Fuels, 2018, 32, 12851-12860.	5.1	14
99	Geometries, electronic properties and stability of molybdenum and tungsten nitrides low-index surfaces. Materials Research Express, 2018, 5, 126402.	1.6	8
100	Hydrodesulfurization of Thiophene over $\text{I}^{\text{III}}\text{-Mo}_2\text{N}$ catalyst. Molecular Catalysis, 2018, 459, 21-30.	2.0	30
101	Modification of Carbon-Based Electroactive Materials for Supercapacitor Applications. , 2018, , 393-413.		3
102	Influence of DC magnetron sputtering reaction gas on structural and optical characteristics of Ce-oxide thin films. Ceramics International, 2018, 44, 16450-16458.	4.8	17
103	Structures and thermodynamic stability of cobalt molybdenum oxide ( $\text{CoMoO}_4\text{-II}$ ). Surface Science, 2018, 677, 52-59.	1.9	9
104	Performance stability of solid-state polypyrrole-reduced graphene oxide-modified carbon bundle fiber for supercapacitor application. Electrochimica Acta, 2018, 285, 9-15.	5.2	25
105	Structural, electronic and thermodynamic properties of bulk and surfaces of terbium dioxide ( $\text{TbO}_2$ ). Materials Research Express, 2018, 5, 085901.	1.6	9
106	Introducing Quantum Chemistry in Chemical Engineering Curriculum. Journal of Chemical Education, 2018, 95, 1562-1571.	2.3	6
107	Bromine fixing ability of electric arc furnace dust during thermal degradation of tetrabromobisphenol: Experimental and thermodynamic analysis study. Journal of Analytical and Applied Pyrolysis, 2018, 134, 503-509.	5.5	14
108	Structural and optical characteristics of pre- and post-annealed sol-gel derived CoCu-oxide coatings. Journal of Alloys and Compounds, 2017, 701, 222-235.	5.5	12

#	ARTICLE	IF	CITATIONS
109	Mechanisms governing selective hydrogenation of acetylene over $\text{Ir}^3\text{-Mo}_2\text{N}$ surfaces. <i>Catalysis Science and Technology</i> , 2017, 7, 943-960.	4.1	25
110	Hydrogen Abstraction from Hydrocarbons by $\text{NH}_2$ . <i>Journal of Physical Chemistry A</i> , 2017, 121, 2221-2231.	2.5	33
111	Reactions of products from thermal degradation of PVC with nanoclusters of $\text{Ir}^{\pm}\text{-Fe}_2\text{O}_3$ (hematite). <i>Chemical Engineering Journal</i> , 2017, 323, 396-405.	12.7	24
112	Reaction of Aniline with Singlet Oxygen ( $\text{O}_2$ $\langle \sup 1 \rangle \langle \sub g \rangle$ ). <i>Journal of Physical Chemistry A</i> , 2017, 121, 3199-3206.	2.5	38
113	Functionalized graphene oxide-reinforced electrospun carbon nanofibers as ultrathin supercapacitor electrode. <i>Journal of Energy Chemistry</i> , 2017, 26, 790-798.	12.9	33
114	Electrospun graphene nanoplatelets-reinforced carbon nanofibers as potential supercapacitor electrode. <i>Materials Letters</i> , 2017, 199, 200-203.	2.6	16
115	Experimental and predicted mechanical properties of $\text{Cr}_x\text{Al}_x\text{N}$ thin films, at high temperatures, incorporating in situ synchrotron radiation X-ray diffraction and computational modelling. <i>RSC Advances</i> , 2017, 7, 22094-22104.	3.6	16
116	Structure, Stability, and (Non)Reactivity of the Low-Index Surfaces of Crystalline $\text{B}_2\text{O}_3$ . <i>Journal of Physical Chemistry C</i> , 2017, 121, 11346-11354.	3.1	10
117	Understanding the adsorptive interactions of arsenate-iron nanoparticles with curved fullerene-like sheets in activated carbon using a quantum mechanics/molecular mechanics computational approach. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 14262-14268.	2.8	4
118	Study of structural properties and defects of Ni-doped $\text{SnO}_2$ nanorods as ethanol gas sensors. <i>Nanotechnology</i> , 2017, 28, 265702.	2.6	23
119	Electrodeposition of Polypyrrole and Reduced Graphene Oxide onto Carbon Bundle Fibre as Electrode for Supercapacitor. <i>Nanoscale Research Letters</i> , 2017, 12, 246.	5.7	79
120	Investigation of the post-annealing electromagnetic response of $\text{Cu}^{\pm}\text{Co}$ oxide coatings via optical measurement and computational modelling. <i>RSC Advances</i> , 2017, 7, 16826-16835.	3.6	27
121	Electronic properties and stability phase diagrams for cubic BN surfaces. <i>Molecular Simulation</i> , 2017, 43, 267-275.	2.0	4
122	Atmospheric oxidation of carbon disulfide ( $\text{CS}_2$ ). <i>Chemical Physics Letters</i> , 2017, 669, 43-48.	2.6	16
123	Formation of PCDDs and PCDFs in the torrefaction of biomass with different chemical composition. <i>Journal of Analytical and Applied Pyrolysis</i> , 2017, 123, 126-133.	5.5	21
124	Green synthesis of mesoporous anatase $\text{TiO}_2$ nanoparticles and their photocatalytic activities. <i>RSC Advances</i> , 2017, 7, 48083-48094.	3.6	118
125	DFT+U and ab initio atomistic thermodynamics approach for mixed transitional metallic oxides: A case study of $\text{CoCu}_2\text{O}_3$ surface terminations. <i>Materials Chemistry and Physics</i> , 2017, 201, 241-250.	4.0	13
126	Enhanced ignition of biomass in presence of $\text{NO}_x$ . <i>Fire Safety Journal</i> , 2017, 91, 235-242.	3.1	4



#	ARTICLE	IF	CITATIONS
127	Flammability of CS <sub>2</sub> and other reduced sulfur species. <i>Fire Safety Journal</i> , 2017, 91, 226-234.	3.1	13
128	Colorimetric and visual dopamine assay based on the use of gold nanorods. <i>Mikrochimica Acta</i> , 2017, 184, 4125-4132.	5.0	17
129	Atmospheric emission of NO from mining explosives: A critical review. <i>Atmospheric Environment</i> , 2017, 167, 81-96.	4.1	38
130	Decomposition of selected chlorinated volatile organic compounds by ceria (CeO <sub>2</sub> ). <i>Catalysis Science and Technology</i> , 2017, 7, 3902-3919.	4.1	64
131	Formation of environmentally-persistent free radicals (EPFR) on $\gamma$ -Al <sub>2</sub> O <sub>3</sub> clusters. <i>RSC Advances</i> , 2017, 7, 52672-52683.	3.6	11
132	Thermal Reduction of NO <sub>x</sub> with Recycled Plastics. <i>Environmental Science &amp; Technology</i> , 2017, 51, 7714-7722.	10.0	15
133	Phenol dissociation on pristine and defective graphene. <i>Surface Science</i> , 2017, 657, 10-14.	1.9	4
134	Understanding the shrinkage of optical absorption edges of nanostructured Cd-Zn sulphide films for photothermal applications. <i>Applied Surface Science</i> , 2017, 392, 854-862.	6.1	33
135	Oxidation of 4-bromo-4'-chlorobiphenyl, model species for forming mixed halogenated aromatic compounds. <i>International Journal of Environment and Pollution</i> , 2017, 61, 243.	0.2	4
136	Chemical bonding states and solar selective characteristics of unbalanced magnetron sputtered Ti <sub>x</sub> M <sub>1-x</sub> N <sub>y</sub> films. <i>RSC Advances</i> , 2016, 6, 36373-36383.	3.6	34
137	Conversion of NO into N <sub>2</sub> over $\beta$ -Mo <sub>2</sub> N. <i>Journal of Physical Chemistry C</i> , 2016, 120, 22270-22280.	3.1	17
138	Formation of Environmentally Persistent Free Radicals on $\gamma$ -Al <sub>2</sub> O <sub>3</sub> . <i>Environmental Science &amp; Technology</i> , 2016, 50, 11094-11102.	10.0	48
139	Large-eddy simulation of methanol pool fires using an accelerated stochastic fields method. <i>Combustion and Flame</i> , 2016, 173, 89-98.	5.2	18
140	New Mechanistic Insights: Why Do Plants Produce Isoprene?. <i>ACS Omega</i> , 2016, 1, 220-225.	3.5	24
141	Thermal Recycling of Brominated Flame Retardants with Fe <sub>2</sub> O <sub>3</sub> . <i>Journal of Physical Chemistry A</i> , 2016, 120, 6039-6047.	2.5	50
142	Structural Thermal Stability of Graphene Oxide-Doped Copper-Cobalt Oxide Coatings as a Solar Selective Surface. <i>Journal of Materials Science and Technology</i> , 2016, 32, 1179-1191.	10.7	24
143	Thermo-elastic and optical properties of molybdenum nitride. <i>Canadian Journal of Physics</i> , 2016, 94, 902-912.	1.1	11
144	Inhibition and Promotion of Pyrolysis by Hydrogen Sulfide (H <sub>2</sub> S) and Sulfanyl Radical (SH). <i>Journal of Physical Chemistry A</i> , 2016, 120, 8941-8948.	2.5	22

#	ARTICLE	IF	CITATIONS
145	NEXAFS N K -edge study of the bonding structure on Al/Si doped sputtered CrN coatings. Journal of Alloys and Compounds, 2016, 661, 268-273.	5.5	13
146	Oxidation of Polyethylene under Corrosive NO <sub>x</sub> Atmosphere. Journal of Physical Chemistry C, 2016, 120, 3766-3775.	3.1	19
147	Effects of annealing temperatures on the morphological, mechanical, surface chemical bonding, and solar selectivity properties of sputtered TiAlSiN thin films. Journal of Alloys and Compounds, 2016, 671, 254-266.	5.5	36
148	Double-sided F and Cl adsorptions on graphene at various atomic ratios: Geometric, orientation and electronic structure aspects. Applied Surface Science, 2016, 373, 65-72.	6.1	13
149	Photodecomposition of bromophenols. Chemosphere, 2016, 150, 749-758.	8.2	18
150	Decomposition of ethylamine through bimolecular reactions. Combustion and Flame, 2016, 163, 532-539.	5.2	23
151	Predicting high temperature mechanical properties of CrN and CrAlN coatings from in-situ synchrotron radiation X-ray diffraction. Thin Solid Films, 2016, 599, 98-103.	1.8	17
152	Interaction of Oxygen with $\sqrt{3}\times\sqrt{3}$ -Rhombohedral Boron (001) Surface. Journal of Physical Chemistry C, 2016, 120, 5968-5979.	3.1	3
153	Trends of elemental adsorption on graphene. Canadian Journal of Physics, 2016, 94, 437-447.	1.1	10
154	Formation of PCDD/Fs in Oxidation of 2-Chlorophenol on Neat Silica Surface. Environmental Science & Technology, 2016, 50, 1412-1418.	10.0	39
155	Thermodynamic Parameters Including Acid Dissociation Constants for Bromochlorophenols (BCPs). Journal of Chemical & Engineering Data, 2016, 61, 160-172.	1.9	2
156	Geometrical and orientational investigations on the electronic structure of graphene with adsorbed aluminium or silicon. Materials and Design, 2016, 89, 27-35.	7.0	6
157	Computational study for the second-stage cracking of the pyrolysis of ethylamine: Decomposition of methanimine, ethenamine, and ethanimine. Computational and Theoretical Chemistry, 2016, 1075, 9-17.	2.5	12
158	Structures, electronic properties and stability phase diagrams for copper( <i>i</i> )/( <i>ii</i> ) bromide surfaces. Physical Chemistry Chemical Physics, 2015, 17, 9341-9351.	2.8	14
159	Formation and Chlorination of Carbazole, Phenoxazine, and Phenazine. Environmental Science & Technology, 2015, 49, 2215-2221.	10.0	65
160	Formation of dibenzofuran, dibenzo-p-dioxin and their hydroxylated derivatives from catechol. Physical Chemistry Chemical Physics, 2015, 17, 1822-1830.	2.8	37
161	Oxidation of crystalline polyethylene. Combustion and Flame, 2015, 162, 3681-3690.	5.2	29
162	Towards a better understanding of the geometrical and orientational aspects of the electronic structure of halogens (F <sup>-</sup> ) adsorption on graphene. Applied Surface Science, 2015, 356, 370-377.	6.1	9

#	ARTICLE	IF	CITATIONS
163	<i>S</i> -Nitrosation of Aminothiones. <i>Journal of Organic Chemistry</i> , 2015, 80, 6951-6958.	3.2	1
164	Formation of polybrominated dibenzofurans from polybrominated biphenyls. <i>Chemosphere</i> , 2015, 119, 1048-1053.	8.2	31
165	Formation of chlorobenzenes by oxidative thermal decomposition of 1,3-dichloropropene. <i>Combustion and Flame</i> , 2015, 162, 2414-2421.	5.2	12
166	Decomposition of S-nitroso species. <i>RSC Advances</i> , 2015, 5, 29914-29923.	3.6	5
167	Formation of mixed halogenated dibenzo-p-dioxins and dibenzofurans (PXDD/Fs). <i>Chemosphere</i> , 2015, 137, 149-156.	8.2	5
168	Reactions of HO <sub>2</sub> with n-propylbenzene and its phenylpropyl radicals. <i>Combustion and Flame</i> , 2015, 162, 1406-1416.	5.2	13
169	Thermal Decomposition of 1,2-Bis(2,4,6-tribromophenoxy)ethane (BTBPE), a Novel Brominated Flame Retardant. <i>Environmental Science &amp; Technology</i> , 2014, 48, 14335-14343.	10.0	51
170	Thermodynamic stability and structures of iron chloride surfaces: A first-principles investigation. <i>Journal of Chemical Physics</i> , 2014, 141, 054709.	3.0	9
171	High level ab initio, DFT, and RRKM calculations for the unimolecular decomposition reaction of ethylamine. <i>Journal of Computational Science</i> , 2014, 5, 568-575.	2.9	16
172	The structures and thermodynamic stability of copper(II) chloride surfaces. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24209-24215.	2.8	13
173	Theoretical insight into chlorine adsorption on the Fe(100) surface. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 8575-8581.	2.8	20
174	Dehydrohalogenation of ethyl halides. <i>Tetrahedron Letters</i> , 2014, 55, 4860-4868.	1.4	36
175	Mechanisms for the formation of polychlorinated dibenzo-p-dioxins and furans (PCDD/Fs) from chlorinated toluenes. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2014, 112, 321-333.	1.7	1
176	Mechanism of Thermal Decomposition of Tetrabromobisphenol A (TBBA). <i>Journal of Physical Chemistry A</i> , 2014, 118, 9338-9346.	2.5	61
177	Mechanisms of transformation of polychlorinated diphenyl ethers into polychlorinated dibenzo-p-dioxins and dibenzofurans. <i>Chemosphere</i> , 2014, 114, 129-135.	8.2	17
178	Quantum Chemical Study on Formation of PCDT/TA from 2-Chlorothiophenol Precursor. <i>Environmental Science &amp; Technology</i> , 2013, 47, 11040-11047.	10.0	21
179	A Mechanistic and Kinetic Study on the Formation of PBDD/Fs from PBDEs. <i>Environmental Science &amp; Technology</i> , 2013, 47, 5118-5127.	10.0	82
180	Theoretical study on the unimolecular decomposition of proline. <i>Computational and Theoretical Chemistry</i> , 2013, 1018, 45-49.	2.5	9

#	ARTICLE	IF	CITATIONS
181	Theoretical investigation into the low-temperature oxidation of ethylbenzene. Proceedings of the Combustion Institute, 2013, 34, 315-323.	3.9	16
182	Formation of polychlorinated dibenzo-p-dioxins and polychlorinated dibenzofurans (PCDD/F) by precursor pathways in oxidation of pesticide alpha-cypermethrin. Proceedings of the Combustion Institute, 2013, 34, 3499-3507.	3.9	7
183	Theoretical study on thermochemical parameters and pKa values for fluorinated isomers of toluene. Computational and Theoretical Chemistry, 2013, 1011, 21-29.	2.5	6
184	Rate constants for reactions of ethylbenzene with hydroperoxyl radical. Combustion and Flame, 2013, 160, 9-16.	5.2	30
185	Theoretical study on thermochemical parameters and IR spectra of chlorinated isomers of nitrobenzene. Canadian Journal of Chemistry, 2013, 91, 999-1008.	1.1	4
186	Density functional theory periodic slab calculations of adsorption and dissociation of H <sub>2</sub> O on the Cu <sub>2</sub> O(110):CuO surface. Canadian Journal of Physics, 2013, 91, 1101-1106.	1.1	10
187	Thermochemical Parameters and p <i>K<sub>a</sub></i> Values for Chlorinated Congeners of Thiophenol. Journal of Chemical & Engineering Data, 2012, 57, 1834-1842.	1.9	14
188	A Mechanistic and Kinetic Study on the Decomposition of Morpholine. Journal of Physical Chemistry A, 2012, 116, 7703-7711.	2.5	12
189	Theoretical study of thermochemical and structural parameters of chlorinated isomers of aniline. Computational and Theoretical Chemistry, 2012, 985, 30-35.	2.5	15
190	Oxidation of dibenzo-p-dioxin: Formation of initial products, 2-methylbenzofuran and 3-hydro-2-methylenebenzofuran. Combustion and Flame, 2012, 159, 3056-3065.	5.2	7
191	Electronic Structure of the CuCl <sub>2</sub> (100) Surface: A DFT First-Principle Study. Journal of Nanomaterials, 2012, 2012, 1-7.	2.7	5
192	Theoretical study on the reaction of the phenoxy radical with O <sub>2</sub> , OH, and NO <sub>2</sub> . International Journal of Quantum Chemistry, 2012, 112, 848-857.	2.0	6
193	A theoretical study on the bimolecular reactions encountered in the pyrolysis of acetamide. Journal of Physical Organic Chemistry, 2012, 25, 431-436.	1.9	5
194	A theoretical study on the pyrolysis of perfluorobutanoic acid as a model compound for perfluoroalkyl acids. Tetrahedron Letters, 2012, 53, 4070-4073.	1.4	21
195	Theoretical Investigation into Competing Unimolecular Reactions Encountered in the Pyrolysis of Acetamide. Journal of Physical Chemistry A, 2011, 115, 14092-14099.	2.5	10
196	Theoretical derivation for reaction rate constants of H abstraction from thiophenol by the H/O radical pool. Computational and Theoretical Chemistry, 2011, 970, 1-5.	2.5	8
197	Theoretical study on the reaction of hydrogen atoms with aniline. Theoretical Chemistry Accounts, 2011, 129, 823-832.	1.4	7
198	Rate constants for hydrogen abstraction reactions by the hydroperoxyl radical from methanol, ethenol, acetaldehyde, toluene, and phenol. Journal of Computational Chemistry, 2011, 32, 1725-1733.	3.3	43

#	ARTICLE	IF	CITATIONS
199	Theoretical study on the unimolecular decomposition of thiophenol. Journal of Computational Chemistry, 2011, 32, 2708-2715.	3.3	7
200	Theoretical study on thermochemical parameters of chlorinated isomers of acetophenone. Computational and Theoretical Chemistry, 2011, 966, 38-43.	2.5	8
201	Formation of polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/F) in oxidation of captan pesticide. Proceedings of the Combustion Institute, 2011, 33, 701-708.	3.9	24
202	A DFT study on the self-coupling reactions of the three isomeric semiquinone radicals. Computational and Theoretical Chemistry, 2010, 958, 106-115.	1.5	9
203	Adsorption of 2-chlorophenol on Cu <sub>2</sub> O(111) – Cu <sub>2</sub> O: A first-principles density functional study. Applied Surface Science, 2010, 256, 4764-4770.	6.1	8
204	Theoretical study of reactions of HO <sub>2</sub> in low-temperature oxidation of benzene. Combustion and Flame, 2010, 157, 1325-1330.	5.2	17
205	Theoretical Study of Unimolecular Decomposition of Catechol. Journal of Physical Chemistry A, 2010, 114, 1060-1067.	2.5	44
206	Theoretical Study of the Ammonia-Hypochlorous Acid Reaction Mechanism. Journal of Physical Chemistry A, 2010, 114, 2597-2606.	2.5	39
207	Theoretical Study on the Thermodynamic Properties and Self-Decomposition of Methylbenzenediol Isomers. Journal of Physical Chemistry A, 2010, 114, 11751-11760.	2.5	4
208	Thermochemical Properties and Decomposition Pathways of Three Isomeric Semiquinone Radicals. Journal of Physical Chemistry A, 2010, 114, 1098-1108.	2.5	36
209	A first-principles density functional study of chlorophenol adsorption on Cu <sub>2</sub> O(110):CuO. Journal of Chemical Physics, 2009, 130, 184505.	3.0	30
210	Mechanisms for formation, chlorination, dechlorination and destruction of polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs). Progress in Energy and Combustion Science, 2009, 35, 245-274.	31.2	401
211	Pyrolysis of permethrin and formation of precursors of polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/F) under non-oxidative conditions. Chemosphere, 2009, 74, 1435-1443.	8.2	32
212	Adsorption of chlorophenol on the Cu(111) surface: A first-principles density functional theory study. Applied Surface Science, 2008, 254, 4218-4224.	6.1	27
213	2-Chlorophenol adsorption on Cu(100): First-principles density functional study. Surface Science, 2008, 602, 1554-1562.	1.9	14
214	Computational Study of the Oxidation and Decomposition of Dibenzofuran under Atmospheric Conditions. Journal of Physical Chemistry A, 2008, 112, 6960-6967.	2.5	30
215	Quantum Chemical and Kinetic Study of Formation of 2-Chlorophenoxy Radical from 2-Chlorophenol: Unimolecular Decomposition and Bimolecular Reactions with H, OH, Cl, and O <sub>2</sub> . Journal of Physical Chemistry A, 2008, 112, 3680-3692.	2.5	34
216	Catalytic Effect of CuO and Other Transition Metal Oxides in Formation of Dioxins: Theoretical Investigation of Reaction Between 2,4,5-Trichlorophenol and CuO. Environmental Science & Technology, 2007, 41, 5708-5715.	10.0	36

#	ARTICLE	IF	CITATIONS
217	Quantum Chemical Investigation of Formation of Polychlorodibenzo-p-Dioxins and Dibenzofurans from Oxidation and Pyrolysis of 2-Chlorophenol. Journal of Physical Chemistry A, 2007, 111, 2563-2573.	2.5	73
218	Theoretical Study of Reaction Pathways of Dibenzofuran and Dibenzo- <i>p</i> -Dioxin under Reducing Conditions. Journal of Physical Chemistry A, 2007, 111, 7133-7140.	2.5	30
219	Quantum Chemical Study of Low Temperature Oxidation Mechanism of Dibenzofuran. Journal of Physical Chemistry A, 2006, 110, 13560-13567.	2.5	29