Thana Maihom

List of Publications by Year
in descending order

66 papers	1,619 citations	257450 24 h-index	315739 38 g-index
67 all docs	67 docs citations	67 times ranked	1896 citing authors

#	Article	IF	Citations
1	Reaction Mechanisms of the Methylation of Ethene with Methanol and Dimethyl Ether over H-ZSM-5: An ONIOM Study. Journal of Physical Chemistry C, 2009, 113, 6654-6662.	3.1	138
2	Reaction Mechanisms for CO Catalytic Oxidation by N₂O on Fe-Embedded Graphene. Journal of Physical Chemistry C, 2012, 116, 16992-16998.	3.1	122
3	Production of Formic Acid via Hydrogenation of CO₂ over a Copper-Alkoxide-Functionalized MOF: A Mechanistic Study. Journal of Physical Chemistry C, 2013, 117, 17650-17658.	3.1	101
4	Effect of the Zeolite Nanocavity on the Reaction Mechanism of n-Hexane Cracking: A Density Functional Theory Study. Journal of Physical Chemistry C, 2010, 114, 7850-7856.	3.1	80
5	Coordinatively Unsaturated Metalâ€“Organic Frameworks M₃(btc)₂ (M = Cr, Fe,) Tj ETQq1 1 0.784314 rgBT / Inorganic Chemistry, 2017, 56, 14005-14012.	4.0	77
6	Halogen substitutions leading to enhanced oxygen evolution and oxygen reduction reactions in metalloporphyrin frameworks. Physical Chemistry Chemical Physics, 2017, 19, 29540-29548.	2.8	59
7	Lithium Bond Impact on Lithium Polysulfide Adsorption with Functionalized Carbon Fiber Paper Interlayers for Lithiumâ€“Sulfur Batteries. Journal of Physical Chemistry C, 2018, 122, 7033-7040.	3.1	55
8	Mechanistic Studies on the Transformation of Ethanol into Ethene over Feâ€ZSMâ€5 Zeolite. ChemPhysChem, 2013, 14, 101-107.	2.1	48
9	Structures and Mechanisms of the Carbonyl-ene Reaction between MOF-11 Encapsulated Formaldehyde and Propylene: An ONIOM Study. Journal of Physical Chemistry C, 2008, 112, 10855-10861.	3.1	47
10	Single-atoms supported (Fe, Co, Ni, Cu) on graphitic carbon nitride for CO2 adsorption and hydrogenation to formic acid: First-principles insights. Applied Surface Science, 2020, 499, 143928.	6.1	47
11	Strong adsorption of lithium polysulfides on ethylenediamine-functionalized carbon fiber paper interlayer providing excellent capacity retention of lithium-sulfur batteries. Carbon, 2017, 123, 492-501.	10.3	42
12	Theoretical Study on Structures and Reaction Mechanisms of Ethylene Oxide Hydration over H-ZSM-5: Ethylene Glycol Formation. Journal of Physical Chemistry C, 2008, 112, 12914-12920.	3.1	40
13	Ethylene Epoxidation with Nitrous Oxide over Feâ€“BTC Metalâ€“Organic Frameworks: A DFT Study. ChemPhysChem, 2016, 17, 3416-3422.	2.1	39
14	Adsorption and decarbonylation of furfural over H-ZSM-5 zeolite: a DFT study. RSC Advances, 2016, 6, 105888-105894.	3.6	37
15	Chiral Macroporous MOF Surfaces for Electroassisted Enantioselective Adsorption and Separation. ACS Applied Materials & Interfaces, 2020, 12, 36548-36557.	8.0	36
16	Collaborative design of Liâ€“S batteries using 3D N-doped graphene aerogel as a sulfur host and graphitic carbon nitride paper as an interlayer. Sustainable Energy and Fuels, 2017, 1, 1759-1765.	4.9	35
17	Chemical Adsorption and Physical Confinement of Polysulfides with the Janus-faced Interlayer for High-performance Lithium-Sulfur Batteries. Scientific Reports, 2017, 7, 17703.	3.3	35
18	Insight into the effect of intercalated alkaline cations of layered manganese oxides on the oxygen reduction reaction and oxygen evolution reaction. Chemical Communications, 2018, 54, 8575-8578.	4.1	33

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19	Density functional study of the activity of gold-supported ZSM-5 zeolites for nitrous oxide decomposition. Chemical Physics Letters, 2013, 556, 217-224.	2.6	29
20	A DFT Study of Tungstenâ€“Methylidene Formation on a W/ZSMâ€5 Zeolite: The Metathesis Active Site. ChemPhysChem, 2015, 16, 3334-3339.	2.1	28
21	Cooperative BrÃ¸nsted-Lewis acid sites created by phosphotungstic acid encapsulated metalâ€“organic frameworks for selective glucose conversion to 5-hydroxymethylfurfural. Fuel, 2022, 310, 122459.	6.4	28
22	Porous Materials as a Platform for Highly Uniform Single-Atom Catalysts: Tuning the Electronic Structure for the Low-Temperature Oxidation of Carbon Monoxide. Journal of Physical Chemistry C, 2016, 120, 19686-19697.	3.1	27
23	Theoretical study on the reaction mechanism of hydrogenation of furfural to furfuryl alcohol on Lewis acidic BEA zeolites: effects of defect structure and tetravalent metals substitution. Physical Chemistry Chemical Physics, 2017, 19, 24042-24048.	2.8	24
24	Computational study of the carbonylâ€“ene reaction between formaldehyde and propylene encapsulated in coordinatively unsaturated metalâ€“organic frameworks M₃(btc)₂ (M = Fe,) Tj ETQq0 0 0 rgBT /Overlock 10	2.8	24
25	First-Principle study of lithium polysulfide adsorption on heteroatom doped graphitic carbon nitride for Lithium-Sulfur batteries. Applied Surface Science, 2021, 565, 150378.	6.1	24
26	Density Functional Theory Study of the Dehydrogenation of Ethanol to Acetaldehyde over the Au-Exchanged ZSM-5 Zeolite: Effect of Surface Oxygen. Journal of Physical Chemistry C, 2014, 118, 18564-18572.	3.1	22
27	Density Functional Investigation of the Conversion of Furfural to Furfuryl Alcohol by Reaction with i-Propanol over UiO-66 Metalâ€“Organic Framework. Inorganic Chemistry, 2021, 60, 4860-4868.	4.0	22
28	Formaldehyde Encapsulated in Lithiumâ€Decorated Metalâ€Organic Frameworks: A Density Functional Theory Study. ChemPhysChem, 2012, 13, 245-249.	2.1	20
29	Furfural to Furfuryl Alcohol: Computational Study of the Hydrogen Transfer on Lewis Acidic BEA Zeolites and Effects of Cation Exchange and Tetravalent Metal Substitution. Inorganic Chemistry, 2018, 57, 6599-6605.	4.0	19
30	Insights into the reaction mechanism of n-hexane dehydroaromatization to benzene over gallium embedded HZSM-5: effect of H₂ incorporated on active sites. Physical Chemistry Chemical Physics, 2019, 21, 5359-5367.	2.8	19
31	Layered manganese oxide nanosheets coated on N-doped graphene aerogel for hydrazine detection: Reaction mechanism investigated by in situ electrochemical X-ray absorption spectroscopy. Journal of Electroanalytical Chemistry, 2018, 808, 124-132.	3.8	18
32	A computational study of the catalytic aerobic epoxidation of propylene over the coordinatively unsaturated metalâ€“organic framework Fe₃(btc)₂: formation of propylene oxide and competing reactions. Physical Chemistry Chemical Physics, 2018, 20, 6726-6734.	2.8	16
33	Theoretical study of CO₂ hydrogenation into formic acid on Lewis acid zeolites. Physical Chemistry Chemical Physics, 2018, 20, 25179-25185.	2.8	16
34	The coumarin synthesis: a combined experimental and theoretical study. Monatshefte FÃ¼r Chemie, 2017, 148, 1245-1250.	1.8	14
35	Highly efficient propane dehydrogenation promoted by reverse waterâ€“gas shift reaction on Pt-Zn alloy surfaces. Fuel, 2022, 325, 124833.	6.4	14
36	Hydration of Carbon Dioxide in Copper-Alkoxide Functionalized Metalâ€“Organic Frameworks: A DFT Study. Journal of Physical Chemistry C, 2015, 119, 3564-3571.	3.1	13

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37	Selective Bond Excision in Nitroimidazoles by Electron Transfer Experiments. Journal of Physical Chemistry A, 2019, 123, 4068-4073.	2.5	13
38	The Activation of Methane on Ru, Rh, and Pd Decorated Carbon Nanotube and Boron Nitride Nanotube: A DFT Study. Catalysts, 2018, 8, 190.	3.5	12
39	Density functional theory study on catalytic cracking of nâ€hexane on heteropoly acid: A comparison with acidic zeolite. Canadian Journal of Chemical Engineering, 2012, 90, 865-872.	1.7	11
40	A proton-hopping charge storage mechanism of ionic one-dimensional coordination polymers for high-performance supercapacitors. Chemical Communications, 2017, 53, 11786-11789.	4.1	11
41	Understanding the interactions between lithium polysulfides and anchoring materials in advanced lithiumâ€“sulfur batteries using density functional theory. Physical Chemistry Chemical Physics, 2022, 24, 8604-8623.	2.8	10
42	Nanocavity effects of various zeolite frameworks on n-pentane cracking to light olefins: combination studies of DFT calculations and experiments. Physical Chemistry Chemical Physics, 2019, 21, 22215-22223.	2.8	9
43	Dehydrogenation of ethanol to acetaldehyde with nitrous oxide over the metalâ€“organic framework NU-1000: a density functional theory study. Physical Chemistry Chemical Physics, 2020, 22, 13622-13628.	2.8	9
44	Theoretical study of methane adsorption and Câ”€H bond activation over Feâ€embedded graphene: Effect of external electric field. Journal of Computational Chemistry, 2019, 40, 2819-2826.	3.3	8
45	Performance of DFT functionals for properties of small molecules containing beryllium, tungsten and hydrogen. Nuclear Materials and Energy, 2020, 22, 100731.	1.3	8
46	A mechanistic study of ethanol transformation into ethene and acetaldehyde on an oxygenated Au-exchanged ZSM-5 zeolite. RSC Advances, 2017, 7, 38052-38058.	3.6	6
47	Insights into glyphosate adsorption on Lewis acidic zeolites from theoretical modelling. Microporous and Mesoporous Materials, 2022, , 112083.	4.4	6
48	Fragmentation of Allylmethylsulfide by Chemical Ionization: Dependence on Humidity and Inhibiting Role of Water. Journal of Physical Chemistry A, 2013, 117, 5149-5160.	2.5	5
49	Theoretical and Experimental Study on the 7â€Hydroxyâ€4â€Methylcoumarin Synthesis with Hâ€Beta Zeolite. ChemistrySelect, 2019, 4, 10660-10667.	1.5	5
50	Phenol Tautomerization Catalyzed by Acidâ€Base Pairs in Lewis Acidic Beta Zeolites: A Computational Study. ChemPhysChem, 2019, 20, 2122-2126.	2.1	5
51	Density functional study of the effect of cation exchanged Sn-Beta zeolite for the diels-alder reaction between furan and methyl acrylate. Chemical Physics Letters, 2020, 754, 137743.	2.6	5
52	Effects of single and double active sites of Cu oxide clusters over the MFI zeolite for direct conversion of methane to methanol: DFT calculations. Physical Chemistry Chemical Physics, 2021, 23, 2500-2510.	2.8	5
53	Modulating the catalytic activity of metal-organic frameworks for CO oxidation with N2O through an oriented external electric field. Molecular Catalysis, 2021, 516, 111970.	2.0	5
54	Adsorption and dehydration of ethanol on isomorphously B, Al, and Ga substituted H-ZSM-5 zeolite: an embedded ONIOM study. Journal of Molecular Modeling, 2021, 27, 354.	1.8	5

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55	Aluminumâ€based Metalâ€Organic Framework as Waterâ€tolerant Lewis Acid Catalyst for Selective Dihydroxyacetone Isomerization to Lactic Acid. ChemCatChem, 2022, 14, .	3.7	5
56	Theoretical insights into furfural reduction to furfuryl alcohol via the catalytic hydrogen transfer reaction catalyzed by cations exchanged zirconium-containing zeolites. Molecular Catalysis, 2021, 504, 111471.	2.0	4
57	The influence of cation exchange and tetravalent metal substitutions in Lewis acidic BEA zeolites for phenol adsorption and Tautomerization: A computational study. Chemical Physics Letters, 2021, 780, 138886.	2.6	4
58	Metal triflate formation of C₁₂â€“C₂₂ phenolic compounds by the simultaneous Câ€“O breaking and Câ€“C coupling of benzyl phenyl ether. Dalton Transactions, 2021, 50, 17390-17396.	3.3	4
59	Mechanism of transfer hydrogenation of carbonyl compounds by zirconium and hafnium-containing metal-organic frameworks. Molecular Catalysis, 2022, 522, 112247.	2.0	4
60	An Experimental and Theoretical Study on the Aldol Condensation on Zirconium-Based Metal-Organic Framework. Key Engineering Materials, 0, 757, 98-102.	0.4	3
61	Effect of Intercalants inside Birnessite-Type Manganese Oxide Nanosheets for Sensor Applications. Inorganic Chemistry, 2020, 59, 15595-15605.	4.0	3
62	Theoretical mechanistic study of the ethylene oxidation over permanganate: effect of BF3 Lewis acid. Monatshefte FÃ¼r Chemie, 2017, 148, 1277-1284.	1.8	2
63	Aluminumâ€Containing Metalâ€Organic Frameworks as Selective and Reusable Catalysts for Glucose Isomerization to Fructose. ChemCatChem, 2022, 14, .	3.7	2
64	Adsorption of Ammonia on Zirconium-Based Metal-Organic Framework: A Combined Experimental and Theoretical Study. Key Engineering Materials, 2017, 757, 93-97.	0.4	1
65	Combined Computational and Experimental Studies of Trans- and Cis-Isomers of Potassium Diaquabis(Oxalato)Chromate (III). Key Engineering Materials, 0, 757, 103-107.	0.4	0
66	Combinations of density functionals for accurate molecular properties of Be/W/H compounds. Nuclear Materials and Energy, 2021, 28, 101026.	1.3	0