

# Thana Maihom

## List of Publications by Year in descending order

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66  
papers

1,619  
citations

257450

24  
h-index

315739

38  
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67  
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67  
docs citations

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times ranked

1896  
citing authors

#	ARTICLE	IF	CITATIONS
1	Cooperative Brønsted-Lewis acid sites created by phosphotungstic acid encapsulated metal-organic frameworks for selective glucose conversion to 5-hydroxymethylfurfural. <i>Fuel</i> , 2022, 310, 122459.	6.4	28
2	Aluminum-based Metal-Organic Framework as Water-tolerant Lewis Acid Catalyst for Selective Dihydroxyacetone Isomerization to Lactic Acid. <i>ChemCatChem</i> , 2022, 14, .	3.7	5
3	Understanding the interactions between lithium polysulfides and anchoring materials in advanced lithium-sulfur batteries using density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 8604-8623.	2.8	10
4	Mechanism of transfer hydrogenation of carbonyl compounds by zirconium and hafnium-containing metal-organic frameworks. <i>Molecular Catalysis</i> , 2022, 522, 112247.	2.0	4
5	Aluminum-Containing Metal-Organic Frameworks as Selective and Reusable Catalysts for Glucose Isomerization to Fructose. <i>ChemCatChem</i> , 2022, 14, .	3.7	2
6	Insights into glyphosate adsorption on Lewis acidic zeolites from theoretical modelling. <i>Microporous and Mesoporous Materials</i> , 2022, , 112083.	4.4	6
7	Highly efficient propane dehydrogenation promoted by reverse water-gas shift reaction on Pt-Zn alloy surfaces. <i>Fuel</i> , 2022, 325, 124833.	6.4	14
8	Effects of single and double active sites of Cu oxide clusters over the MFI zeolite for direct conversion of methane to methanol: DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2500-2510.	2.8	5
9	Theoretical insights into furfural reduction to furfuryl alcohol via the catalytic hydrogen transfer reaction catalyzed by cations exchanged zirconium-containing zeolites. <i>Molecular Catalysis</i> , 2021, 504, 111471.	2.0	4
10	Density Functional Investigation of the Conversion of Furfural to Furfuryl Alcohol by Reaction with <i>i</i> -Propanol over UiO-66 Metal-Organic Framework. <i>Inorganic Chemistry</i> , 2021, 60, 4860-4868.	4.0	22
11	Combinations of density functionals for accurate molecular properties of Be/W/H compounds. <i>Nuclear Materials and Energy</i> , 2021, 28, 101026.	1.3	0
12	The influence of cation exchange and tetravalent metal substitutions in Lewis acidic BEA zeolites for phenol adsorption and Tautomerization: A computational study. <i>Chemical Physics Letters</i> , 2021, 780, 138886.	2.6	4
13	First-Principle study of lithium polysulfide adsorption on heteroatom doped graphitic carbon nitride for Lithium-Sulfur batteries. <i>Applied Surface Science</i> , 2021, 565, 150378.	6.1	24
14	Modulating the catalytic activity of metal-organic frameworks for CO oxidation with N <sub>2</sub> O through an oriented external electric field. <i>Molecular Catalysis</i> , 2021, 516, 111970.	2.0	5
15	Metal triflate formation of C <sub>12</sub> -C <sub>22</sub> phenolic compounds by the simultaneous C-O breaking and C-C coupling of benzyl phenyl ether. <i>Dalton Transactions</i> , 2021, 50, 17390-17396.	3.3	4
16	Adsorption and dehydration of ethanol on isomorphously B, Al, and Ga substituted H-ZSM-5 zeolite: an embedded ONIOM study. <i>Journal of Molecular Modeling</i> , 2021, 27, 354.	1.8	5
17	Single-atoms supported (Fe, Co, Ni, Cu) on graphitic carbon nitride for CO <sub>2</sub> adsorption and hydrogenation to formic acid: First-principles insights. <i>Applied Surface Science</i> , 2020, 499, 143928.	6.1	47
18	Chiral Macroporous MOF Surfaces for Electroassisted Enantioselective Adsorption and Separation. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 36548-36557.	8.0	36

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19	Effect of Intercalants inside Birnessite-Type Manganese Oxide Nanosheets for Sensor Applications. <i>Inorganic Chemistry</i> , 2020, 59, 15595-15605.	4.0	3
20	Dehydrogenation of ethanol to acetaldehyde with nitrous oxide over the metal-organic framework NU-1000: a density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 13622-13628.	2.8	9
21	Performance of DFT functionals for properties of small molecules containing beryllium, tungsten and hydrogen. <i>Nuclear Materials and Energy</i> , 2020, 22, 100731.	1.3	8
22	Density functional study of the effect of cation exchanged Sn-Beta zeolite for the diels-alder reaction between furan and methyl acrylate. <i>Chemical Physics Letters</i> , 2020, 754, 137743.	2.6	5
23	Theoretical study of methane adsorption and C-H bond activation over Fe-embedded graphene: Effect of external electric field. <i>Journal of Computational Chemistry</i> , 2019, 40, 2819-2826.	3.3	8
24	Theoretical and Experimental Study on the 7-Hydroxy-4-Methylcoumarin Synthesis with H-Beta Zeolite. <i>ChemistrySelect</i> , 2019, 4, 10660-10667.	1.5	5
25	Nanocavity effects of various zeolite frameworks on <i>n</i> -pentane cracking to light olefins: combination studies of DFT calculations and experiments. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22215-22223.	2.8	9
26	Insights into the reaction mechanism of <i>n</i> -hexane dehydroaromatization to benzene over gallium embedded HZSM-5: effect of H <sub>2</sub> incorporated on active sites. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 5359-5367.	2.8	19
27	Computational study of the carbonyl-ene reaction between formaldehyde and propylene encapsulated in coordinatively unsaturated metal-organic frameworks M <sub>3</sub> (btc) <sub>2</sub> (M = Fe, Tj ETQq1.1.0.784314 rgBT /	1.0	14
28	Phenol Tautomerization Catalyzed by Acid-Base Pairs in Lewis Acidic Beta Zeolites: A Computational Study. <i>ChemPhysChem</i> , 2019, 20, 2122-2126.	2.1	5
29	Selective Bond Excision in Nitroimidazoles by Electron Transfer Experiments. <i>Journal of Physical Chemistry A</i> , 2019, 123, 4068-4073.	2.5	13
30	A computational study of the catalytic aerobic epoxidation of propylene over the coordinatively unsaturated metal-organic framework Fe <sub>3</sub> (btc) <sub>2</sub> : formation of propylene oxide and competing reactions. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 6726-6734.	2.8	16
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. <i>Journal of Electroanalytical Chemistry</i> , 2018, 808, 124-132.	3.8	18
32	Lithium Bond Impact on Lithium Polysulfide Adsorption with Functionalized Carbon Fiber Paper Interlayers for Lithium-Sulfur Batteries. <i>Journal of Physical Chemistry C</i> , 2018, 122, 7033-7040.	3.1	55
33	Insight into the effect of intercalated alkaline cations of layered manganese oxides on the oxygen reduction reaction and oxygen evolution reaction. <i>Chemical Communications</i> , 2018, 54, 8575-8578.	4.1	33
34	Furfural to Furfuryl Alcohol: Computational Study of the Hydrogen Transfer on Lewis Acidic BEA Zeolites and Effects of Cation Exchange and Tetravalent Metal Substitution. <i>Inorganic Chemistry</i> , 2018, 57, 6599-6605.	4.0	19
35	Theoretical study of CO <sub>2</sub> hydrogenation into formic acid on Lewis acid zeolites. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25179-25185.	2.8	16
36	The Activation of Methane on Ru, Rh, and Pd Decorated Carbon Nanotube and Boron Nitride Nanotube: A DFT Study. <i>Catalysts</i> , 2018, 8, 190.	3.5	12

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37	The coumarin synthesis: a combined experimental and theoretical study. <i>Monatshefte für Chemie</i> , 2017, 148, 1245-1250.	1.8	14
38	Coordinatively Unsaturated Metal-Organic Frameworks $M_3(btc)_2$ (M = Cr, Fe.) <i>Inorganic Chemistry</i> , 2017, 56, 14005-14012.	4.0	77
39	Adsorption of Ammonia on Zirconium-Based Metal-Organic Framework: A Combined Experimental and Theoretical Study. <i>Key Engineering Materials</i> , 2017, 757, 93-97.	0.4	1
40	A proton-hopping charge storage mechanism of ionic one-dimensional coordination polymers for high-performance supercapacitors. <i>Chemical Communications</i> , 2017, 53, 11786-11789.	4.1	11
41	Halogen substitutions leading to enhanced oxygen evolution and oxygen reduction reactions in metalloporphyrin frameworks. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29540-29548.	2.8	59
42	Collaborative design of Li-S batteries using 3D N-doped graphene aerogel as a sulfur host and graphitic carbon nitride paper as an interlayer. <i>Sustainable Energy and Fuels</i> , 2017, 1, 1759-1765.	4.9	35
43	Strong adsorption of lithium polysulfides on ethylenediamine-functionalized carbon fiber paper interlayer providing excellent capacity retention of lithium-sulfur batteries. <i>Carbon</i> , 2017, 123, 492-501.	10.3	42
44	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. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 24042-24048.	2.8	24
45	A mechanistic study of ethanol transformation into ethene and acetaldehyde on an oxygenated Au-exchanged ZSM-5 zeolite. <i>RSC Advances</i> , 2017, 7, 38052-38058.	3.6	6
46	Theoretical mechanistic study of the ethylene oxidation over permanganate: effect of BF <sub>3</sub> Lewis acid. <i>Monatshefte für Chemie</i> , 2017, 148, 1277-1284.	1.8	2
47	Chemical Adsorption and Physical Confinement of Polysulfides with the Janus-faced Interlayer for High-performance Lithium-Sulfur Batteries. <i>Scientific Reports</i> , 2017, 7, 17703.	3.3	35
48	Ethylene Epoxidation with Nitrous Oxide over Fe-BTC Metal-Organic Frameworks: A DFT Study. <i>ChemPhysChem</i> , 2016, 17, 3416-3422.	2.1	39
49	Porous Materials as a Platform for Highly Uniform Single-Atom Catalysts: Tuning the Electronic Structure for the Low-Temperature Oxidation of Carbon Monoxide. <i>Journal of Physical Chemistry C</i> , 2016, 120, 19686-19697.	3.1	27
50	Adsorption and decarbonylation of furfural over H-ZSM-5 zeolite: a DFT study. <i>RSC Advances</i> , 2016, 6, 105888-105894.	3.6	37
51	A DFT Study of Tungsten-Methylidene Formation on a W/ZSM-5 Zeolite: The Metathesis Active Site. <i>ChemPhysChem</i> , 2015, 16, 3334-3339.	2.1	28
52	Hydration of Carbon Dioxide in Copper-Alkoxide Functionalized Metal-Organic Frameworks: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 3564-3571.	3.1	13
53	Density Functional Theory Study of the Dehydrogenation of Ethanol to Acetaldehyde over the Au-Exchanged ZSM-5 Zeolite: Effect of Surface Oxygen. <i>Journal of Physical Chemistry C</i> , 2014, 118, 18564-18572.	3.1	22
54	Production of Formic Acid via Hydrogenation of CO <sub>2</sub> over a Copper-Alkoxide-Functionalized MOF: A Mechanistic Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 17650-17658.	3.1	101

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55	Mechanistic Studies on the Transformation of Ethanol into Ethene over Fe-ZSM-5 Zeolite. ChemPhysChem, 2013, 14, 101-107.	2.1	48
56	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
57	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
58	Reaction Mechanisms for CO Catalytic Oxidation by N <sub>2</sub> O on Fe-Embedded Graphene. Journal of Physical Chemistry C, 2012, 116, 16992-16998.	3.1	122
59	Density functional theory study on catalytic cracking of <i>n</i> -hexane on heteropoly acid: A comparison with acidic zeolite. Canadian Journal of Chemical Engineering, 2012, 90, 865-872.	1.7	11
60	Formaldehyde Encapsulated in Lithium-Decorated Metal-Organic Frameworks: A Density Functional Theory Study. ChemPhysChem, 2012, 13, 245-249.	2.1	20
61	Effect of the Zeolite Nanocavity on the Reaction Mechanism of <i>n</i> -Hexane Cracking: A Density Functional Theory Study. Journal of Physical Chemistry C, 2010, 114, 7850-7856.	3.1	80
62	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
63	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
64	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
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	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