

# Debmalya Ray

## List of Publications by Year in descending order

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Version: 2024-02-01

26  
papers

1,249  
citations

516561

16  
h-index

580701

25  
g-index

26  
all docs

26  
docs citations

26  
times ranked

2025  
citing authors

#	ARTICLE	IF	CITATIONS
1	Methane Oxidation to Methanol Catalyzed by Cu-Oxo Clusters Stabilized in NU-1000 Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2017, 139, 10294-10301.	6.6	282
2	Machine learning the quantum-chemical properties of metal-organic frameworks for accelerated materials discovery. <i>Matter</i> , 2021, 4, 1578-1597.	5.0	170
3	A porous, electrically conductive hexa-zirconium( $\mu_4$ ) metal-organic framework. <i>Chemical Science</i> , 2018, 9, 4477-4482.	3.7	158
4	Tuning Catalytic Sites on $Zr_6O_8$ Metal-Organic Framework Nodes via Ligand and Defect Chemistry Probed with <i>tert</i> -Butyl Alcohol Dehydration to Isobutylene. <i>Journal of the American Chemical Society</i> , 2020, 142, 8044-8056.	6.6	83
5	From Transition Metals to Lanthanides to Actinides: Metal-Mediated Tuning of Electronic Properties of Isostructural Metal-Organic Frameworks. <i>Inorganic Chemistry</i> , 2018, 57, 13246-13251.	1.9	80
6	Computational Study of Structural and Electronic Properties of Lead-Free $CsMl_3$ Perovskites (M = Ge, Sn, Pb, Mg, Ca, Sr, and Ba). <i>Journal of Physical Chemistry C</i> , 2018, 122, 7838-7848.	1.5	62
7	Elucidating bonding preferences in tetrakis(imido)uranate(VI) dianions. <i>Nature Chemistry</i> , 2017, 9, 850-855.	6.6	54
8	Insights into the Structure-Activity Relationships in Metal-Organic Framework-Supported Nickel Catalysts for Ethylene Hydrogenation. <i>ACS Catalysis</i> , 2020, 10, 8995-9005.	5.5	40
9	Advancement of Actinide Metal-Organic Framework Chemistry via Synthesis of Pu-UiO-66. <i>Journal of the American Chemical Society</i> , 2020, 142, 9363-9371.	6.6	38
10	In Situ Formation of Unprecedented Neptunium-Oxide Wheel Clusters Stabilized in a Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2019, 141, 11842-11846.	6.6	36
11	Photocatalytic Biocidal Coatings Featuring $Zr_6Ti_4$ -Based Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2022, 144, 12192-12201.	6.6	35
12	Metal-Organic Frameworks with Metal-Catecholates for $O_2/N_2$ Separation. <i>Journal of Physical Chemistry C</i> , 2019, 123, 12935-12946.	1.5	33
13	$Cu[Ni(2,3\text{-pyrazinedithiolate})_2]$ Metal-Organic Framework for Electrocatalytic Hydrogen Evolution. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 34419-34427.	4.0	23
14	Sulfur Vacancy Clustering and Its Impact on Electronic Properties in Pyrite $FeS_2$ . <i>Chemistry of Materials</i> , 2020, 32, 4820-4831.	3.2	21
15	Precise Control of Cu Nanoparticle Size and Catalytic Activity through Pore Templating in Zr Metal-Organic Frameworks. <i>Chemistry of Materials</i> , 2020, 32, 3078-3086.	3.2	21
16	Using Redox-Active Ligands to Generate Actinide Ligand Radical Species. <i>Inorganic Chemistry</i> , 2021, 60, 15242-15252.	1.9	19
17	Exploring the Effects of Node Topology, Connectivity, and Metal Identity on the Binding of Nerve Agents and Their Hydrolysis Products in Metal-Organic Frameworks. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 35657-35675.	4.0	17
18	Tuning the Conductivity of Hexa-Zirconium(IV) Metal-Organic Frameworks by Encapsulating Heterofullerenes. <i>Chemistry of Materials</i> , 2021, 33, 1182-1189.	3.2	17

#	ARTICLE	IF	CITATIONS
19	Leveraging Nitrogen Linkages in the Formation of a Porous Thorium-Organic Nanotube Suitable for Iodine Capture. <i>Inorganic Chemistry</i> , 2022, 61, 9480-9492.	1.9	14
20	The Role of the Organic Solvent Polarity in Isolating Uranyl Peroxide Capsule Fragments. <i>Inorganic Chemistry</i> , 2020, 59, 1633-1641.	1.9	11
21	Flying onto global minima on potential energy surfaces: A swarm intelligence guided route to molecular electronic structure. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25328.	1.0	10
22	Experimental and Quantum Mechanical Characterization of an Oxygen-Bridged Plutonium(IV) Dimer. <i>Chemistry - A European Journal</i> , 2020, 26, 8115-8120.	1.7	9
23	Neptunyl Peroxide Chemistry: Synthesis and Spectroscopic Characterization of a Neptunyl Triperoxide Compound, $\text{Ca}_2[\text{NpO}_2(\text{O})_3] \cdot 9\text{H}_2\text{O}$ . <i>Inorganic Chemistry</i> , 2019, 58, 12264-12271.	1.9	6
24	Electron transitions in a Ce(III)-catecholate metal-organic framework. <i>Chemical Communications</i> , 2022, 58, 525-528.	2.2	5
25	Mitigation of the internal p-n junction in $\text{CoS}_2$ -contacted $\text{FeS}_2$ single crystals: Assessing bulk semiconducting transport. <i>Physical Review Materials</i> , 2021, 5,	0.9	4
26	Unsaturated Sulfur Crown Ethers Can Extract Mercury(II) and Show Promise for Future Copernicium(II) Studies: A Combined Experimental and Computational Study. <i>Inorganic Chemistry</i> , 2022, 61, 807-817.	1.9	1