## Daniele Ongari

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Data-Driven Matching of Experimental Crystal Structures and Gas Adsorption Isotherms of Metal–Organic Frameworks. Journal of Chemical & Engineering Data, 2022, 67, 1743-1756.	1.0	6
2	Pyrene-based metal organic frameworks: from synthesis to applications. Chemical Society Reviews, 2021, 50, 3143-3177.	18.7	126
3	Using collective knowledge to assign oxidation states of metal cations in metal–organic frameworks. Nature Chemistry, 2021, 13, 771-777.	6.6	35
4	Diversifying Databases of Metal Organic Frameworks for High-Throughput Computational Screening. ACS Applied Materials & Interfaces, 2021, 13, 61004-61014.	4.0	50
5	Too Many Materials and Too Many Applications: An Experimental Problem Waiting for a Computational Solution. ACS Central Science, 2020, 6, 1890-1900.	5.3	63
6	Understanding the diversity of the metal-organic framework ecosystem. Nature Communications, 2020, 11, 4068.	5.8	282
7	Thermoelasticity of Flexible Organic Crystals from Quasi-harmonic Lattice Dynamics: The Case of Copper(II) Acetylacetonate. Journal of Physical Chemistry Letters, 2020, 11, 8543-8548.	2.1	15
8	Big-Data Science in Porous Materials: Materials Genomics and Machine Learning. Chemical Reviews, 2020, 120, 8066-8129.	23.0	284
9	In Silico Discovery of Covalent Organic Frameworks for Carbon Capture. ACS Applied Materials & Interfaces, 2020, 12, 21559-21568.	4.0	43
10	Metal-organic frameworks as kinetic modulators for branched selectivity in hydroformylation. Nature Communications, 2020, 11, 1059.	5.8	40
11	Metal Organic Frameworks for Xenon Storage Applications. , 2020, 2, 233-238.		10
12	Can Metal–Organic Frameworks Be Used for Cannabis Breathalyzers?. ACS Applied Materials & Interfaces, 2019, 11, 34777-34786.	4.0	1
13	Applicability of Tail Corrections in the Molecular Simulations of Porous Materials. Journal of Chemical Theory and Computation, 2019, 15, 5635-5641.	2.3	30
14	Building a Consistent and Reproducible Database for Adsorption Evaluation in Covalent–Organic Frameworks. ACS Central Science, 2019, 5, 1663-1675.	5.3	89
15	Evaluating Charge Equilibration Methods To Generate Electrostatic Fields in Nanoporous Materials. Journal of Chemical Theory and Computation, 2019, 15, 382-401.	2.3	70
16	Photocatalytic hydrogen generation from a visible-light responsive metal–organic framework system: the impact of nickel phosphide nanoparticles. Journal of Materials Chemistry A, 2018, 6, 2476-2481.	5.2	94
17	Biporous Metal–Organic Framework with Tunable CO <sub>2</sub> /CH <sub>4</sub> Separation Performance Facilitated by Intrinsic Flexibility. ACS Applied Materials & Interfaces, 2018, 10, 36144-36156.	4.0	33
18	Photocatalytic Hydrogen Generation from a Visible-Light-Responsive Metal–Organic Framework System: Stability versus Activity of Molybdenum Sulfide Cocatalysts. ACS Applied Materials & Interfaces, 2018, 10, 30035-30039.	4.0	71

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#	Article	IF	CITATIONS
19	Xenon Recovery at Room Temperature using Metal–Organic Frameworks. Chemistry - A European Journal, 2017, 23, 10758-10762.	1.7	38
20	Metal–Organic Frameworks Invert Molecular Reactivity: Lewis Acidic Phosphonium Zwitterions Catalyze the Aldol-Tishchenko Reaction. Journal of the American Chemical Society, 2017, 139, 18166-18169.	6.6	30
21	Accurate Characterization of the Pore Volume in Microporous Crystalline Materials. Langmuir, 2017, 33, 14529-14538.	1.6	155
22	Origin of the Strong Interaction between Polar Molecules and Copper(II) Paddle-Wheels in Metal Organic Frameworks. Journal of Physical Chemistry C, 2017, 121, 15135-15144.	1.5	23