Diego A GÃ³mez-GualdrÃ³n

List of Publications by Year
in descending order

53 papers	4,979 citations	172457 29 h-index	175258 52 g-index
56 all docs	56 docs citations	56 times ranked	5590 citing authors

#	Article	IF	Citations
1	Discovery of spontaneous de-interpenetration through charged point-point repulsions. CheM, 2022, 8, 225-242.	11.7	11
2	Energetics of Reaction Pathways Enabled by N and H Radicals during Catalytic, Plasma-Assisted NH₃ Synthesis. ACS Sustainable Chemistry and Engineering, 2022, 10, 2034-2051.	6.7	24
3	High-Throughput Experimentation for Selective Growth of Small-Diameter Single-Wall Carbon Nanotubes Using Ru-Promoted Co Catalysts. Chemistry of Materials, 2022, 34, 4548-4559.	6.7	2
4	Stacking of Monolayer Graphene Particles at a Waterâ€“Vapor Interface. Journal of Physical Chemistry C, 2021, 125, 7880-7888.	3.1	7
5	Deep learning combined with IAST to screen thermodynamically feasible MOFs for adsorption-based separation of multiple binary mixtures. Journal of Chemical Physics, 2021, 154, 234102.	3.0	17
6	Exploiting hydrophobicity and hydrophilicity in nanopores as a design principle for â€œsmartâ€•MOF microtanks for methane storage. Molecular Systems Design and Engineering, 2020, 5, 166-176.	3.4	4
7	Adsorption Isotherm Predictions for Multiple Molecules in MOFs Using the Same Deep Learning Model. Journal of Chemical Theory and Computation, 2020, 16, 1271-1283.	5.3	76
8	Electronic effects due to organic linker-metal surface interactions: implications on screening of MOF-encapsulated catalysts. Physical Chemistry Chemical Physics, 2020, 22, 2475-2487.	2.8	10
9	Vacancy Healing as a Desorption Tool: Oxygen Triggered Removal of Stored Ammonia from NiO_{1â€“x}/MOR Validated by Experiments and Simulations. ACS Applied Energy Materials, 2020, 3, 8233-8239.	5.1	6
10	Large-Scale Free Energy Calculations on a Computational Metalâ€“Organic Frameworks Database: Toward Synthetic Likelihood Predictions. Chemistry of Materials, 2020, 32, 8106-8119.	6.7	24
11	Balancing volumetric and gravimetric uptake in highly porous materials for clean energy. Science, 2020, 368, 297-303.	12.6	429
12	Improving Energy Transfer within Metalâ€“Organic Frameworks by Aligning Linker Transition Dipoles along the Framework Axis. Journal of the American Chemical Society, 2020, 142, 11192-11202.	13.7	48
13	Material Consequences of Hydrogen Dissolution in Palladium Alloys Observed from First Principles. Journal of Physical Chemistry C, 2019, 123, 22158-22171.	3.1	8
14	Modular Synthesis of Highly Porous Zr-MOFs Assembled from Simple Building Blocks for Oxygen Storage. ACS Applied Materials & Interfaces, 2019, 11, 42179-42185.	8.0	17
15	Increasing topological diversity during computational â€œsynthesisâ€•of porous crystals: how and why. CrystEngComm, 2019, 21, 1653-1665.	2.6	69
16	Structure-Mechanical Stability Relations of Metal-Organic Frameworks via Machine Learning. Matter, 2019, 1, 219-234.	10.0	170
17	Dissociation, Dissolution, and Diffusion of Nitrogen on V_xFe_y and V_xCr_y Alloy Membranes Studied by First Principles. Journal of Physical Chemistry C, 2019, 123, 30416-30426.	3.1	1
18	Attainable Volumetric Targets for Adsorption-Based Hydrogen Storage in Porous Crystals: Molecular Simulation and Machine Learning. Journal of Physical Chemistry C, 2019, 123, 120-130.	3.1	57

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19	Benchmark Study of Hydrogen Storage in Metalâ€“Organic Frameworks under Temperature and Pressure Swing Conditions. ACS Energy Letters, 2018, 3, 748-754.	17.4	147
20	Time Dependent Structural Evolution of Porous Organic Cage CC3. Crystal Growth and Design, 2018, 18, 921-927.	3.0	19
21	Molecular Simulation Insights on Xe/Kr Separation in a Set of Nanoporous Crystalline Membranes. ACS Applied Materials & Interfaces, 2018, 10, 582-592.	8.0	44
22	Hierarchically Engineered Mesoporous Metal-Organic Frameworks toward Cell-free Immobilized Enzyme Systems. CheM, 2018, 4, 1022-1034.	11.7	281
23	Molecular Building Block-Based Electronic Charges for High-Throughput Screening of Metalâ€“Organic Frameworks for Adsorption Applications. Journal of Chemical Theory and Computation, 2018, 14, 365-376.	5.3	18
24	Role of Pore Chemistry and Topology in the CO₂ Capture Capabilities of MOFs: From Molecular Simulation to Machine Learning. Chemistry of Materials, 2018, 30, 6325-6337.	6.7	144
25	Impact of the strength and spatial distribution of adsorption sites on methane deliverable capacity in nanoporous materials. Chemical Engineering Science, 2017, 159, 18-30.	3.8	26
26	Bottom-up construction of a superstructure in a porous uranium-organic crystal. Science, 2017, 356, 624-627.	12.6	286
27	Understanding Volumetric and Gravimetric Hydrogen Adsorption Trade-off in Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2017, 9, 33419-33428.	8.0	104
28	G-quadruplex organic frameworks. Nature Chemistry, 2017, 9, 466-472.	13.6	99
29	Elucidating the Nanoparticleâ€“Metal Organic Framework Interface of Pt@ZIF-8 Catalysts. Journal of Physical Chemistry C, 2017, 121, 25079-25091.	3.1	28
30	Topologically Guided, Automated Construction of Metalâ€“Organic Frameworks and Their Evaluation for Energy-Related Applications. Crystal Growth and Design, 2017, 17, 5801-5810.	3.0	176
31	Evaluating topologically diverse metalâ€“organic frameworks for cryo-adsorbed hydrogen storage. Energy and Environmental Science, 2016, 9, 3279-3289.	30.8	231
32	Nanosizing a Metalâ€“Organic Framework Enzyme Carrier for Accelerating Nerve Agent Hydrolysis. ACS Nano, 2016, 10, 9174-9182.	14.6	202
33	CO₂ adsorption-induced structural changes in coordination polymer ligands elucidated via molecular simulations and experiments. Dalton Transactions, 2016, 45, 17168-17178.	3.3	11
34	In silico discovery of metal-organic frameworks for precombustion CO ₂ capture using a genetic algorithm. Science Advances, 2016, 2, e1600909.	10.3	231
35	Framework-Topology-Dependent Catalytic Activity of Zirconium-Based (Porphinato)zinc(II) MOFs. Journal of the American Chemical Society, 2016, 138, 14449-14457.	13.7	210
36	Implications of sterically constrained n-butane oxidation reactions on the reaction mechanism and selectivity to 1-butanol. Surface Science, 2016, 653, 11-21.	1.9	5

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37	Application of Consistency Criteria To Calculate BET Areas of Micro- And Mesoporous Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2016, 138, 215-224.	13.7	201
38	The materials genome in action: identifying the performance limits for methane storage. Energy and Environmental Science, 2015, 8, 1190-1199.	30.8	314
39	Ultrahigh Surface Area Zirconium MOFs and Insights into the Applicability of the BET Theory. Journal of the American Chemical Society, 2015, 137, 3585-3591.	13.7	329
40	A modelling approach for MOF-encapsulated metal catalysts and application to n-butane oxidation. Physical Chemistry Chemical Physics, 2015, 17, 27596-27608.	2.8	19
41	Ultraporous, Water Stable, and Breathing Zirconium-Based Metalâ€“Organic Frameworks with ftw Topology. Journal of the American Chemical Society, 2015, 137, 13183-13190.	13.7	149
42	Computational Design of Metalâ€“Organic Frameworks Based on Stable Zirconium Building Units for Storage and Delivery of Methane. Chemistry of Materials, 2014, 26, 5632-5639.	6.7	191
43	Waterâ€Stable Zirconiumâ€Based Metalâ€“Organic Framework Material with Highâ€Surface Area and Gasâ€Storage Capacities. Chemistry - A European Journal, 2014, 20, 12389-12393.	3.3	150
44	Isoreticular Series of (3,24)-Connected Metalâ€“Organic Frameworks: Facile Synthesis and High Methane Uptake Properties. Chemistry of Materials, 2014, 26, 1912-1917.	6.7	76
45	Exploring the Limits of Methane Storage and Delivery in Nanoporous Materials. Journal of Physical Chemistry C, 2014, 118, 6941-6951.	3.1	108
46	Characterization of carbon atomistic pathways during single-walled carbon nanotube growth on supported metal nanoparticles. Carbon, 2013, 57, 298-309.	10.3	23
47	Effects of Precursor Type on the CVD Growth of Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2013, 117, 10397-10409.	3.1	18
48	Characterization of Metal Nanocatalyst State and Morphology during Simulated Single-Walled Carbon Nanotube Growth. Journal of Physical Chemistry C, 2013, 117, 12061-12070.	3.1	13
49	Dynamic Evolution of Supported Metal Nanocatalyst/Carbon Structure during Single-Walled Carbon Nanotube Growth. ACS Nano, 2012, 6, 720-735.	14.6	55
50	Growth of chiral single-walled carbon nanotube caps in the presence of a cobalt cluster. Nanotechnology, 2009, 20, 215601.	2.6	18
51	Effect of Metal Cluster-Cap Interactions on the Catalyzed Growth of Single-Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2009, 113, 698-709.	3.1	32
52	The role of cap chirality in the mechanism of growth of single-wall carbon nanotubes. Nanotechnology, 2008, 19, 485604.	2.6	37
53	A self-assembling, biporous, metal-binding covalent organic framework and its application for gas separation. Materials Advances, 0, , .	5.4	3