Juan JosÃ© GutiÃ©rrez-Sevillano

List of Publications by Year
in descending order

42 papers	1,368 citations	279701 23 h-index	330025 37 g-index
42 all docs	42 docs citations	42 times ranked	2014 citing authors

#	Article	IF	Citations
1	Understanding Gas-Induced Structural Deformation of ZIF-8. Journal of Physical Chemistry Letters, 2012, 3, 1159-1164.	2.1	143
2	Effect of Room-Temperature Ionic Liquids on CO₂ Separation by a Cu-BTC Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2013, 117, 20762-20768.	1.5	84
3	Molecular Mechanisms for Adsorption in Cu-BTC Metal Organic Framework. Journal of Physical Chemistry C, 2013, 117, 11357-11366.	1.5	81
4	Zeolite screening for the separation of gas mixtures containing SO₂, CO₂and CO. Physical Chemistry Chemical Physics, 2014, 16, 19884.	1.3	81
5	Understanding Adsorption of Highly Polar Vapors on Mesoporous MIL-100(Cr) and MIL-101(Cr): Experiments and Molecular Simulations. Journal of Physical Chemistry C, 2013, 117, 7613-7622.	1.5	79
6	High Adsorption Capacities and Two-Step Adsorption of Polar Adsorbates on Copperâ€“Benzene-1,3,5-tricarboxylate Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2013, 117, 18100-18111.	1.5	67
7	Solubility of the Precombustion Gases CO₂, CH₄, CO, H₂, N₂, and H₂S in the Ionic Liquid [bmim][Tf₂N] from Monte Carlo Simulations. Journal of Physical Chemistry C, 2014, 118, 23599-23604.	1.5	67
8	Enantioselective adsorption of ibuprofen and lysine in metalâ€“organic frameworks. Chemical Communications, 2014, 50, 10849.	2.2	52
9	Adsorption of hydrogen sulphide on Metal-Organic Frameworks. RSC Advances, 2013, 3, 14737.	1.7	49
10	Analysis of the ITQ-12 Zeolite Performance in Propaneâˆ’Propylene Separations Using a Combination of Experiments and Molecular Simulations. Journal of Physical Chemistry C, 2010, 114, 14907-14914.	1.5	47
11	Modeling Gas Adsorption in Flexible Metalâ€“Organic Frameworks via Hybrid Monte Carlo/Molecular Dynamics Schemes. Advanced Theory and Simulations, 2019, 2, 1800177.	1.3	40
12	Role of Ionic Liquid [EMIM]⁺[SCN]^{âˆ’} in the Adsorption and Diffusion of Gases in Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2018, 10, 29694-29704.	4.0	38
13	Methane Adsorption in Zr-Based MOFs: Comparison and Critical Evaluation of Force Fields. Journal of Physical Chemistry C, 2017, 121, 25309-25322.	1.5	34
14	Insights on the Molecular Mechanisms of Hydrogen Adsorption in Zeolites. Journal of Physical Chemistry C, 2013, 117, 14374-14380.	1.5	33
15	Molecular dynamics simulations of organohalide perovskite precursors: solvent effects in the formation of perovskite solar cells. Physical Chemistry Chemical Physics, 2015, 17, 22770-22777.	1.3	32
16	Transferable force fields for adsorption of small gases in zeolites. Physical Chemistry Chemical Physics, 2015, 17, 24048-24055.	1.3	30
17	How ligands improve the hydrothermal stability and affect the adsorption in the IRMOF family. Physical Chemistry Chemical Physics, 2013, 15, 17696.	1.3	29
18	Selective Adsorption of Water from Mixtures with 1-Alcohols by Exploitation of Molecular Packing Effects in CuBTC. Journal of Physical Chemistry C, 2015, 119, 3658-3666.	1.5	29

#	Article	IF	Citations
19	Validation of the CO₂/N₂O Analogy Using Molecular Simulation. Industrial & Engineering Chemistry Research, 2014, 53, 18081-18090.	1.8	28
20	Water adsorption in ideal and defective UiO-66 structures. Microporous and Mesoporous Materials, 2022, 330, 111555.	2.2	28
21	Molecular simulation investigation into the performance of Cuâ€“BTC metalâ€“organic frameworks for carbon dioxideâ€“methane separations. Physical Chemistry Chemical Physics, 2011, 13, 20453.	1.3	25
22	Toward a Transferable Set of Charges to Model Zeolitic Imidazolate Frameworks: Combined Experimentalâ€“Theoretical Research. Journal of Physical Chemistry C, 2013, 117, 466-471.	1.5	24
23	Strategies to Simultaneously Enhance the Hydrostability and the Alcoholâ€“Water Separation Behavior of Cu-BTC. Journal of Physical Chemistry C, 2013, 117, 20706-20714.	1.5	23
24	Simulation Study of Structural Changes in Zeolite RHO. Journal of Physical Chemistry C, 2013, 117, 11592-11599.	1.5	23
25	Zeolites for the selective adsorption of sulfur hexafluoride. Physical Chemistry Chemical Physics, 2015, 17, 18121-18130.	1.3	22
26	Critical Role of Dynamic Flexibility in Geâ€Containing Zeolites: Impact on Diffusion. Chemistry - A European Journal, 2016, 22, 10036-10043.	1.7	22
27	Separation of benzene from mixtures with water, methanol, ethanol, and acetone: highlighting hydrogen bonding and molecular clustering influences in CuBTC. Physical Chemistry Chemical Physics, 2015, 17, 20114-20124.	1.3	20
28	Adsorptive separation of ethane and ethylene using IsoReticular Metal-Organic Frameworks. Microporous and Mesoporous Materials, 2017, 248, 40-45.	2.2	20
29	Identifying Zeolite Topologies for Storage and Release of Hydrogen. Journal of Physical Chemistry C, 2018, 122, 12485-12493.	1.5	20
30	Carbon Dioxide Capture Enhanced by Preâ€Adsorption of Water and Methanol in UiOâ€66. Chemistry - A European Journal, 2021, 27, 14653-14659.	1.7	17
31	A Simulation Study of Hydrogen in Metalâ€“Organic Frameworks. Adsorption Science and Technology, 2010, 28, 823-835.	1.5	14
32	Effect of the molecular interactions on the separation of nonpolar mixtures using Cu-BTC metalâ€“organic framework. Microporous and Mesoporous Materials, 2013, 165, 79-83.	2.2	13
33	Macroscopic and Microscopic View of Competitive and Cooperative Adsorption of Alcohol Mixtures on ZIF-8. Langmuir, 2019, 35, 3887-3896.	1.6	11
34	Separation of Amyl Alcohol Isomers in ZIFâ€77. ChemPhysChem, 2015, 16, 2735-2738.	1.0	8
35	Effect of Light Gases in the Ethane/Ethylene Separation Using Zeolitic Imidazolate Frameworks. Journal of Physical Chemistry C, 2018, 122, 8637-8646.	1.5	8
36	Metastable Zr/Hf-MOFs: the hexagonal family of EHU-30 and their water-sorption induced structural transformation. Inorganic Chemistry Frontiers, 2021, 8, 4767-4779.	3.0	8

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37	OCEAN: An Algorithm to Predict the Separation of Biogas Using Zeolites. Industrial & Engineering Chemistry Research, 2020, 59, 7212-7223.	1.8	7
38	COSMO-3D: Incorporating Three-Dimensional Contact Information into the COSMO-SAC Model. Industrial & Engineering Chemistry Research, 2015, 54, 2214-2226.	1.8	5
39	Modifying the hydrophobic nature of MAF-6. Separation and Purification Technology, 2021, 277, 119422.	3.9	3
40	Computational Approaches to Zeolite-Based Adsorption Processes. Structure and Bonding, 2020, , 57-83.	1.0	2
41	Using Aliphatic Alcohols to Tune Benzene Adsorption in MAFâ€6. Advanced Theory and Simulations, 2019, 2, 1900112.	1.3	1
42	On the design of models for an accurate description of the water â€“ hematite interface. Applied Surface Science, 2021, 560, 149884.	3.1	1