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	Water adsorption in ideal and defective UiO-66 structures. Microporous and Mesoporous Materials, 2022, 330, 111555.	2.2	28
2	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
3	On the design of models for an accurate description of the water â€“ hematite interface. Applied Surface Science, 2021, 560, 149884.	3.1	1
4	Modifying the hydrophobic nature of MAF-6. Separation and Purification Technology, 2021, 277, 119422.	3.9	3
5	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
6	Computational Approaches to Zeolite-Based Adsorption Processes. Structure and Bonding, 2020, , 57-83.	1.0	2
7	OCEAN: An Algorithm to Predict the Separation of Biogas Using Zeolites. Industrial & Engineering Chemistry Research, 2020, 59, 7212-7223.	1.8	7
8	Using Aliphatic Alcohols to Tune Benzene Adsorption in MAFâ€6. Advanced Theory and Simulations, 2019, 2, 1900112.	1.3	1
9	Macroscopic and Microscopic View of Competitive and Cooperative Adsorption of Alcohol Mixtures on ZIF-8. Langmuir, 2019, 35, 3887-3896.	1.6	11
10	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
11	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
12	Identifying Zeolite Topologies for Storage and Release of Hydrogen. Journal of Physical Chemistry C, 2018, 122, 12485-12493.	1.5	20
13	Role of Ionic Liquid [EMIM]⁺[SCN]^{â^'} in the Adsorption and Diffusion of Gases in Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2018, 10, 29694-29704.	4.0	38
14	Adsorptive separation of ethane and ethylene using IsoReticular Metal-Organic Frameworks. Microporous and Mesoporous Materials, 2017, 248, 40-45.	2.2	20
15	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
16	Critical Role of Dynamic Flexibility in Geâ€Containing Zeolites: Impact on Diffusion. Chemistry - A European Journal, 2016, 22, 10036-10043.	1.7	22
17	Separation of Amyl Alcohol Isomers in ZIFâ€7. ChemPhysChem, 2015, 16, 2735-2738.	1.0	8
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

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19	COSMO-3D: Incorporating Three-Dimensional Contact Information into the COSMO-SAC Model. Industrial & Engineering Chemistry Research, 2015, 54, 2214-2226.	1.8	5
20	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
21	Zeolites for the selective adsorption of sulfur hexafluoride. Physical Chemistry Chemical Physics, 2015, 17, 18121-18130.	1.3	22
22	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
23	Transferable force fields for adsorption of small gases in zeolites. Physical Chemistry Chemical Physics, 2015, 17, 24048-24055.	1.3	30
24	Validation of the CO₂/N₂O Analogy Using Molecular Simulation. Industrial & Engineering Chemistry Research, 2014, 53, 18081-18090.	1.8	28
25	Zeolite screening for the separation of gas mixtures containing SO₂, CO₂and CO. Physical Chemistry Chemical Physics, 2014, 16, 19884.	1.3	81
26	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
27	Enantioselective adsorption of ibuprofen and lysine in metalâ€“organic frameworks. Chemical Communications, 2014, 50, 10849.	2.2	52
28	Adsorption of hydrogen sulphide on Metal-Organic Frameworks. RSC Advances, 2013, 3, 14737.	1.7	49
29	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
30	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
31	How ligands improve the hydrothermal stability and affect the adsorption in the IRMOF family. Physical Chemistry Chemical Physics, 2013, 15, 17696.	1.3	29
32	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
33	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
34	Molecular Mechanisms for Adsorption in Cu-BTC Metal Organic Framework. Journal of Physical Chemistry C, 2013, 117, 11357-11366.	1.5	81
35	Simulation Study of Structural Changes in Zeolite RHO. Journal of Physical Chemistry C, 2013, 117, 11592-11599.	1.5	23
36	Insights on the Molecular Mechanisms of Hydrogen Adsorption in Zeolites. Journal of Physical Chemistry C, 2013, 117, 14374-14380.	1.5	33

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37	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
38	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
39	Understanding Gas-Induced Structural Deformation of ZIF-8. Journal of Physical Chemistry Letters, 2012, 3, 1159-1164.	2.1	143
40	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
41	A Simulation Study of Hydrogen in Metalâ€“Organic Frameworks. Adsorption Science and Technology, 2010, 28, 823-835.	1.5	14
42	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