Santiago Builes

List of Publications by Year
in descending order

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21 papers	737 citations	471509 17 h-index	752698 20 g-index
21 all docs	21 docs citations	21 times ranked	961 citing authors

#	Article	IF	Citations
1	Isosteric Heats of Gas and Liquid Adsorption. Langmuir, 2013, 29, 10416-10422.	3.5	100
2	A Semiempirical Method to Detect and Correct DFT-Based Gas-Phase Errors and Its Application in Electrocatalysis. ACS Catalysis, 2020, 10, 6900-6907.	11.2	71
3	A brief review of the computational modeling of CO2 electroreduction on Cu electrodes. Current Opinion in Electrochemistry, 2018, 9, 158-165.	4.8	64
4	Microporous carbon adsorbents with high CO2 capacities for industrial applications. Physical Chemistry Chemical Physics, 2011, 13, 16063.	2.8	53
5	Substantial improvement of electrocatalytic predictions by systematic assessment of solvent effects on adsorption energies. Applied Catalysis B: Environmental, 2020, 276, 119147.	20.2	53
6	Effect of Immobilized Amines on the Sorption Properties of Solid Materials: Impregnation versus Grafting. Langmuir, 2013, 29, 199-206.	3.5	44
7	Optimization of the separation of sulfur hexafluoride and nitrogen by selective adsorption using monte carlo simulations. AICHE Journal, 2011, 57, 962-974.	3.6	42
8	Understanding CO₂ Capture in Amine-Functionalized MCM-41 by Molecular Simulation. Journal of Physical Chemistry C, 2012, 116, 3017-3024.	3.1	40
9	Adsorption of Cadmium Using Biochars Produced from Agro-Residues. Journal of Physical Chemistry C, 2020, 124, 14592-14602.	3.1	37
10	Analysis of CO₂ Adsorption in Amine-Functionalized Porous Silicas by Molecular Simulations. Energy & Fuels, 2015, 29, 3855-3862.	5.1	36
11	How symmetry factors cause potential- and facet-dependent pathway shifts during CO2 reduction to CH4 on Cu electrodes. Applied Catalysis B: Environmental, 2021, 285, 119776.	20.2	28
12	Alkylsilane-Functionalized Microporous and Mesoporous Materials: Molecular Simulation and Experimental Analysis of Gas Adsorption. Journal of Physical Chemistry C, 2012, 116, 10150-10161.	3.1	25
13	Understanding the Performance of New Amine-Functionalized Mesoporous Silica Materials for CO₂ Adsorption. Industrial & Engineering Chemistry Research, 2014, 53, 15611-15619.	3.7	25
14	Hybrid aminopolymerâ€“silica materials for efficient CO₂adsorption. RSC Advances, 2015, 5, 104943-104953.	3.6	22
15	Fast Correction of Errors in the DFTâ€Calculated Energies of Gaseous Nitrogenâ€Containing Species. ChemCatChem, 2021, 13, 2508-2516.	3.7	21
16	A Comparative Assessment of Emerging Solvents and Adsorbents for Mitigating CO2 Emissions From the Industrial Sector by Using Molecular Modeling Tools. Frontiers in Energy Research, 2020, 8, .	2.3	20
17	Impact of Intrinsic Density Functional Theory Errors on the Predictive Power of Nitrogen Cycle Electrocatalysis Models. ACS Catalysis, 2022, 12, 4784-4791.	11.2	20
18	Influence of Van der Waals Interactions on the Solvation Energies of Adsorbates at Ptâ€Based Electrocatalysts. ChemPhysChem, 2019, 20, 2968-2972.	2.1	16

#	Article	IF	Citations
19	Effect of Amine Functionalization of MOF Adsorbents for Enhanced CO2 Capture and Separation: A Molecular Simulation Study. Frontiers in Chemistry, 2020, 8, 574622.	3.6	16
20	Predictions of fluidities of amines by molecular simulations: TraPPE-EH vs. OPLS-AA. Fluid Phase Equilibria, 2018, 464, 40-46.	2.5	4
21	Resistance to Grinding and Cement Paste Performance of Blends of Clinker, Limestone and Gypsum. Journal of the Institution of Engineers (India): Series A, 2021, 102, 535-543.	1.2	0