Santiago Builes

List of Publications by Year
in descending order

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Version: 2024-02-01

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	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
2	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
3	Fast Correction of Errors in the DFTâ€Calculated Energies of Gaseous Nitrogenâ€Containing Species. ChemCatChem, 2021, 13, 2508-2516.	3.7	21
4	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
5	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
6	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
7	Adsorption of Cadmium Using Biochars Produced from Agro-Residues. Journal of Physical Chemistry C, 2020, 124, 14592-14602.	3.1	37
8	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
9	Substantial improvement of electrocatalytic predictions by systematic assessment of solvent effects on adsorption energies. Applied Catalysis B: Environmental, 2020, 276, 119147.	20.2	53
10	Influence of Van der Waals Interactions on the Solvation Energies of Adsorbates at Ptâ€Based Electrocatalysts. ChemPhysChem, 2019, 20, 2968-2972.	2.1	16
11	Predictions of fluidities of amines by molecular simulations: TraPPE-EH vs. OPLS-AA. Fluid Phase Equilibria, 2018, 464, 40-46.	2.5	4
12	A brief review of the computational modeling of CO2 electroreduction on Cu electrodes. Current Opinion in Electrochemistry, 2018, 9, 158-165.	4.8	64
13	Hybrid aminopolymerâ€“silica materials for efficient CO₂adsorption. RSC Advances, 2015, 5, 104943-104953.	3.6	22
14	Analysis of CO₂ Adsorption in Amine-Functionalized Porous Silicas by Molecular Simulations. Energy & Fuels, 2015, 29, 3855-3862.	5.1	36
15	Understanding the Performance of New Amine-Functionalized Mesoporous Silica Materials for CO₂ Adsorption. Industrial & Engineering Chemistry Research, 2014, 53, 15611-15619.	3.7	25
16	Isosteric Heats of Gas and Liquid Adsorption. Langmuir, 2013, 29, 10416-10422.	3.5	100
17	Effect of Immobilized Amines on the Sorption Properties of Solid Materials: Impregnation versus Grafting. Langmuir, 2013, 29, 199-206.	3.5	44
18	Understanding CO₂ Capture in Amine-Functionalized MCM-41 by Molecular Simulation. Journal of Physical Chemistry C, 2012, 116, 3017-3024.	3.1	40

#	Article	IF	Citations
19	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
20	Microporous carbon adsorbents with high CO2 capacities for industrial applications. Physical Chemistry Chemical Physics, 2011, 13, 16063.	2.8	53
21	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