Daniel Bahamon

List of Publications by Year
in descending order

40 papers	955 citations	471371 17 h-index	454834 30 g-index
40 all docs	40 docs citations	40 times ranked	932 citing authors

#	Article	IF	Citations
1	Modifying absorption process configurations to improve their performance for Post-Combustion CO2 capture â€“ What have we learned and what is still Missing?. Chemical Engineering Journal, 2022, 430, 133096.	6.6	34
2	Molecular Thermodynamic Modeling of Hybrid Ionic Liquids for Biogas Upgrading. Industrial & Engineering Chemistry Research, 2022, 61, 12190-12207.	1.8	1
3	Insights into the thermal stability and conversion of carbon-based materials by using ReaxFF reactive force field: Recent advances and future directions. Carbon, 2022, 196, 840-866.	5.4	32
4	Adhesion and Cohesion of Silica Surfaces with Quartz Cement: A Molecular Simulations Study. ACS Omega, 2022, 7, 22303-22316.	1.6	2
5	Insights into the performance of hybrid graphene oxide/MOFs for CO2 capture at process conditions by molecular simulations. Chemical Engineering Journal, 2022, 449, 137884.	6.6	10
6	Understanding the relationship between the structural properties of three corrosion inhibitors and their surface protectiveness ability in different environments. Applied Surface Science, 2021, 542, 148600.	3.1	25
7	A DFT study of the adsorption energy and electronic interactions of the SO₂ molecule on a CoP hydrotreating catalyst. RSC Advances, 2021, 11, 2947-2957.	1.7	49
8	Are we missing something when evaluating adsorbents for CO₂ capture at the system level?. Energy and Environmental Science, 2021, 14, 6360-6380.	15.6	16
9	Systematic Search of Suitable Metalâ€“Organic Frameworks for Thermal Energy-Storage Applications with Low Global Warming Potential Refrigerants. ACS Sustainable Chemistry and Engineering, 2021, 9, 3157-3171.	3.2	15
10	Grand Canonical Monte Carlo Simulations to Determine the Optimal Interlayer Distance of a Graphene Slit-Shaped Pore for Adsorption of Methane, Hydrogen and their Equimolar Mixture. Nanomaterials, 2021, 11, 2534.	1.9	5
11	Current and future perspectives on catalytic-based integrated carbon capture and utilization. Science of the Total Environment, 2021, 790, 148081.	3.9	67
12	Sustainability criteria as a game changer in the search for hybrid solvents for CO2 and H2S removal. Separation and Purification Technology, 2021, 277, 119516.	3.9	11
13	How Molecular Modelling Tools Can Help in Mitigating Climate Change. Molecular Modeling and Simulation, 2021, , 181-220.	0.2	2
14	Computational modeling of green hydrogen generation from photocatalytic H2S splitting: Overview and perspectives. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2021, 49, 100456.	5.6	15
15	Surface modification of antiâ€fouling novel cellulose/graphene oxide (GO) nanosheets (NS) microfiltration membranes for seawater desalination applications. Journal of Chemical Technology and Biotechnology, 2020, 95, 1915-1925.	1.6	26
16	Perspectives and guidelines on thermodynamic modelling of deep eutectic solvents. Journal of Molecular Liquids, 2020, 298, 112183.	2.3	83
17	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, .	1.2	20
18	Screening of Ionic Liquids and Deep Eutectic Solvents for Physical CO₂ Absorption by Soft-SAFT Using Key Performance Indicators. Journal of Chemical & Engineering Data, 2020, 65, 5844-5861.	1.0	40

#	Article	IF	Citations
19	Design of Subâ€Nanochannels between Graphene Oxide Sheets via Crown Ether Intercalation to Selectively Regulate Cation Permeation. Advanced Materials Interfaces, 2020, 7, 1901876.	1.9	17
20	Performance of Activated Carbons Derived from Date Seeds in CO₂ Swing Adsorption Determined by Combining Experimental and Molecular Simulation Data. Industrial & Engineering Chemistry Research, 2020, 59, 7161-7173.	1.8	25
21	Effect of Amine Functionalization of MOF Adsorbents for Enhanced CO2 Capture and Separation: A Molecular Simulation Study. Frontiers in Chemistry, 2020, 8, 574622.	1.8	16
22	Assessing the Feasibility of Deep Eutectic Solvents For CO2 Capture From Molecular And Process Modeling. , 2020, , .		0
23	Insights into the Transport Properties of Electrolyte Solutions in a Hierarchical Carbon Electrode by Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2019, 123, 27273-27285.	1.5	11
24	Molecular simulations of phenol and ibuprofen removal from water using multilayered graphene oxide membranes. Molecular Physics, 2019, 117, 3703-3714.	0.8	15
25	Molecular simulations of carbon-based materials for selected CO2 separation and water treatment processes. Fluid Phase Equilibria, 2019, 492, 10-25.	1.4	19
26	Energetic evaluation of swing adsorption processes for CO 2 capture in selected MOFs and zeolites: Effect of impurities. Chemical Engineering Journal, 2018, 342, 458-473.	6.6	76
27	Density Functional Theory-Based Adsorption Isotherms for Pure and Flue Gas Mixtures on Mg-MOF-74. Application in CO₂ Capture Swing Adsorption Processes. Journal of Physical Chemistry C, 2018, 122, 3945-3957.	1.5	38
28	Computational study of ibuprofen removal from water by adsorption in realistic activated carbons. Journal of Colloid and Interface Science, 2017, 498, 323-334.	5.0	64
29	Optimal Faujasite structures for post combustion CO 2 capture and separation in different swing adsorption processes. Journal of CO2 Utilization, 2017, 19, 100-111.	3.3	35
30	Computational simulation study of the influence of faujasite Si/Al ratio on CO2 capture by temperature swing adsorption. Journal of CO2 Utilization, 2017, 21, 261-269.	3.3	16
31	Pharmaceutical Removal from Water Effluents by Adsorption on Activated Carbons: A Monte Carlo Simulation Study. Langmuir, 2017, 33, 11146-11155.	1.6	36
32	Pharmaceuticals removal from water effluents by adsorption in activated carbons using Monte Carlo simulations. Computer Aided Chemical Engineering, 2017, 40, 2695-2700.	0.3	11
33	Comparative Study of MOFs and Zeolites For CO2 Capture and Separation at Process Conditions. , 2016, , .		3
34	Systematic evaluation of materials for post-combustion CO 2 capture in a Temperature Swing Adsorption process. Chemical Engineering Journal, 2016, 284, 438-447.	6.6	118
35	Synergetic Effect of Physicochemical and Electrostatic Strategies on Ion Sieving for Polymer Cross-linked Graphene Oxide Membrane. Environmental Science: Nano, 0, , .	2.2	2
36	Design of Novel Hybrid Adsorption Processes for CO ₂ Capture Using an Integrated Multi-Scale Modelling. SSRN Electronic Journal, 0, , .	0.4	0

#	Article	IF	Citations
37	Thermodynamic and Process Modeling of Deep Eutectic Solvents for CO2 Capture and Separation at Industrial Condition. SSRN Electronic Journal, 0, , .	0.4	0
38	Molecular Design of Novel Carbon-Based Materials for CO ₂ Capture by Swing Adsorption Processes. SSRN Electronic Journal, 0, , .	0.4	0
39	Design and Optimization of Processes with Novel Adsorbent Materials for Co2 Capture by a Combined Molecular Simulations-Experimental Approach. SSRN Electronic Journal, 0, , .	0.4	0
40	Robust Thermodynamic Models to Describe the Physicochemical Behaviour of Deep Eutectic Solvents for Gas Separation. , 0, , .		0