Alfredo Mj SÃ¡nchez De MerÃ¡s

List of Publications by Year
in descending order

15 papers	1,912 citations	840776 11 h-index	996975 15 g-index
15 all docs	15 docs citations	15 times ranked	2194 citing authors

#	Article	IF	Citations
1	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.	4.1	5
2	Flexibility in the Graphene Sheet: The Influence on Gas Adsorption from Molecular Dynamics Studies. Journal of Physical Chemistry C, 2019, 123, 28035-28047.	3.1	14
3	Molecular Dynamics of CH4/N2 Mixtures on a Flexible Graphene Layer: Adsorption and Selectivity Case Study. Frontiers in Chemistry, 2019, 7, 386.	3.6	14
4	Modeling the Interaction of Carbon Monoxide with Flexible Graphene: From Coupled Cluster Calculations to Molecularâ€Dynamics Simulations. ChemPhysChem, 2018, 19, 774-783.	2.1	23
5	Potential models for the simulation of methane adsorption on graphene: development and CCSD(T) benchmarks. Physical Chemistry Chemical Physics, 2018, 20, 25518-25530.	2.8	23
6	Nitrogen Gas on Graphene: Pairwise Interaction Potentials. Lecture Notes in Computer Science, 2018, , 563-578.	1.3	3
7	Modelization of the $$hbox {H}_{2}$$ H 2 adsorption on graphene and molecular dynamics simulation. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	6
8	MP2 Study of Physisorption of Molecular Hydrogen onto Defective Nanotubes: Cooperative Effect in Stoneâ€“Wales Defects. Journal of Physical Chemistry A, 2016, 120, 4951-4960.	2.5	13
9	Multi-level coupled cluster theory. Journal of Chemical Physics, 2014, 141, 224105.	3.0	45
10	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
11	The CCSD(T) model with Cholesky decomposition of orbital energy denominators. International Journal of Quantum Chemistry, 2011, 111, 349-355.	2.0	11
12	Cholesky decomposition-based definition of atomic subsystems in electronic structure calculations. Journal of Chemical Physics, 2010, 132, 204105.	3.0	22
13	Fast noniterative orbital localization for large molecules. Journal of Chemical Physics, 2006, 125, 174101.	3.0	138
14	Reduced scaling in electronic structure calculations using Cholesky decompositions. Journal of Chemical Physics, 2003, 118, 9481-9484.	3.0	386
15	Size-intensive decomposition of orbital energy denominators. Journal of Chemical Physics, 2000, 113, 508-513.	3.0	43