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	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
2	Reduced scaling in electronic structure calculations using Cholesky decompositions. Journal of Chemical Physics, 2003, 118, 9481-9484.	3.0	386
3	Fast noniterative orbital localization for large molecules. Journal of Chemical Physics, 2006, 125, 174101.	3.0	138
4	Multi-level coupled cluster theory. Journal of Chemical Physics, 2014, 141, 224105.	3.0	45
5	Size-intensive decomposition of orbital energy denominators. Journal of Chemical Physics, 2000, 113, 508-513.	3.0	43
6	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
7	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
8	Cholesky decomposition-based definition of atomic subsystems in electronic structure calculations. Journal of Chemical Physics, 2010, 132, 204105.	3.0	22
9	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
10	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
11	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
12	The CCSD(T) model with Cholesky decomposition of orbital energy denominators. International Journal of Quantum Chemistry, 2011, 111, 349-355.	2.0	11
13	Modelization of the $$hbox {H}_{2}$$ H 2 adsorption on graphene and molecular dynamics simulation. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	6
14	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
15	Nitrogen Gas on Graphene: Pairwise Interaction Potentials. Lecture Notes in Computer Science, 2018, , 563-578.	1.3	3