Juan F Espinal

List of Publications by Year
in descending order

25 papers	1,085 citations	759233 12 h-index	610901 24 g-index
26 all docs	26 docs citations	26 times ranked	1404 citing authors

#	Article	IF	Citations
1	Improving the deconvolution and interpretation of XPS spectra from chars by ab initio calculations. Carbon, 2016, 110, 155-171.	10.3	351
2	Structural analysis of char by Raman spectroscopy: Improving band assignments through computational calculations from first principles. Carbon, 2016, 100, 678-692.	10.3	288
3	A DFT Study of Interaction of Carbon Monoxide with Carbonaceous Materials. Journal of Physical Chemistry B, 2004, 108, 1003-1008.	2.6	74
4	Thermodynamic evaluation of steam gasification mechanisms of carbonaceous materials. Carbon, 2009, 47, 3010-3018.	10.3	47
5	Mechanisms of NH3 formation during the reaction of H2 with nitrogen containing carbonaceous materials. Carbon, 2007, 45, 2273-2279.	10.3	44
6	Experimental characterization and molecular simulation of nitrogen complexes formed upon NOâ€“char reaction at 270 Â°C in the presence of H2O and O2. Carbon, 2004, 42, 1507-1515.	10.3	41
7	Mechanisms for methane and ethane formation in the reaction of hydrogen with carbonaceous materials. Carbon, 2005, 43, 1820-1827.	10.3	36
8	Molecular Interaction of (Ethanol)2â^'Water Heterotrimers. Journal of Physical Chemistry A, 2007, 111, 8250-8256.	2.5	31
9	Effect of calcium on gasification of carbonaceous materials with CO2: A DFT study. Fuel, 2013, 114, 199-205.	6.4	30
10	Theoretical Study of Sodium Effect on the Gasification of Carbonaceous Materials with Carbon Dioxide. Journal of Physical Chemistry A, 2015, 119, 12756-12766.	2.5	27
11	Cooperative effects on the structure and stability of (ethanol)3â€“water, (methanol)3â€“water heterotetramers and (ethanol)4, (methanol)4 tetramers. Computational and Theoretical Chemistry, 2009, 901, 186-193.	1.5	26
12	Mechanisms for homogeneous and heterogeneous formation of methane during the carbonâ€“hydrogen reaction over zigzag edge sites. Carbon, 2016, 102, 390-402.	10.3	26
13	Understanding the kinetics of carbon-hydrogen reaction: Insights from reaction mechanisms on zigzag edges for homogeneous and heterogeneous formation of methane. Carbon, 2017, 118, 597-606.	10.3	12
14	Experimental and Computational Analysis of the Formation of Surface Oxygen Functional Groups during Iron Catalyzed Char Gasification with CO2. Combustion Science and Technology, 2018, 190, 687-706.	2.3	10
15	Calcination Temperature Effect in Catalyst Reactivity for the CO SELOX Reaction Using Perovskite-like LaBO3 (B: Mn, Fe, Co, Ni) Oxides. Catalysis Letters, 2021, 151, 3690-3703.	2.6	7
16	The role of OHâ€¦O and CHâ€¦O hydrogen bonds and Hâ€¦H interactions in ethanol/methanolâ€“water heterohexamers. Journal of Molecular Modeling, 2016, 22, 181.	1.8	6
17	Thermochemistry and kinetic analysis for the conversion of furfural to valuable added products. Journal of Molecular Modeling, 2019, 25, 26.	1.8	6
18	Thermodynamic evaluation of carbon dioxide gasification reactions at oxy-combustion conditions. Combustion Science and Technology, 2018, 190, 1515-1527.	2.3	5

#	Article	IF	Citations
19	Prediction of 1,3,5-triisopropylbenzene cracking pattern through thermodynamic evaluation of products and protonation intermediates. Molecular Catalysis, 2019, 466, 13-18.	2.0	5
20	Exploration of the (ethanol)₄â€“water heteropentamers potential energy surface by simulated annealing and Ab initio molecular dynamics. International Journal of Quantum Chemistry, 2011, 111, 3080-3096.	2.0	4
21	Looking for the Azeotrope: A Computational Study of (Ethanol)6â€“Water, (Methanol)6â€“Water, (Ethanol)7, and (Methanol)7 Heptamers. Journal of Physical Chemistry A, 2020, 124, 7080-7087.	2.5	4
22	Double-walled carbon nanotube deformation by interacting with a nickel surface: A DFT study. Computational Materials Science, 2020, 174, 109457.	3.0	2
23	HeteropentÃ¡meros (etanol)4-agua: estudio estructural y termodinÃ¡mico. Quimica Nova, 2010, 33, 860-866.	0.3	1
24	Mechanisms of Carbon Gasification Reactions Using Electronic Structure Methods. , 2011, , 445-501.		1
25	CO Oxidation Catalytic Effects of Intrinsic Surface Defects in Rhombohedral LaMnO₃. ChemPhysChem, 2022, 23, e202200152.	2.1	1