Angeles Pulido

List of Publications by Year
in descending order

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34 papers	2,371 citations	257450 24 h-index	377865 34 g-index
34 all docs	34 docs citations	34 times ranked	3229 citing authors

#	Article	IF	Citations
1	Photocatalytic proton reduction by a computationally identified, molecular hydrogen-bonded framework. Journal of Materials Chemistry A, 2020, 8, 7158-7170.	10.3	45
2	From Concept to Crystals via Prediction: Multiâ€Component Organic Cage Pots by Social Selfâ€Sorting. Angewandte Chemie, 2019, 131, 16421-16427.	2.0	23
3	From Concept to Crystals via Prediction: Multiâ€Component Organic Cage Pots by Social Selfâ€Sorting. Angewandte Chemie - International Edition, 2019, 58, 16275-16281.	13.8	52
4	Applications of crystal structure prediction â€“ organic molecular structures: general discussion. Faraday Discussions, 2018, 211, 493-539.	3.2	8
5	Near-Ideal Xylene Selectivity in Adaptive Molecular Pillar[n]arene Crystals. Journal of the American Chemical Society, 2018, 140, 6921-6930.	13.7	191
6	Computationally-Guided Synthetic Control over Pore Size in Isostructural Porous Organic Cages. ACS Central Science, 2017, 3, 734-742.	11.3	68
7	Functional materials discovery using energyâ€“structureâ€“function maps. Nature, 2017, 543, 657-664.	27.8	348
8	Reticular synthesis of porous molecular 1D nanotubes and 3D networks. Nature Chemistry, 2017, 9, 17-25.	13.6	122
9	Effect of the C_{Î±} substitution on the ketonic decarboxylation of carboxylic acids over m-ZrO₂: the role of entropy. Catalysis Science and Technology, 2016, 6, 5561-5566.	4.1	13
10	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	1.1	445
11	Rigid/Flexible Organic Structure Directing Agents for Directing the Synthesis of Multipore Zeolites: A Computational Approach. Journal of Physical Chemistry C, 2015, 119, 7711-7720.	3.1	13
12	Propene epoxidation with O₂or H₂â€“O₂mixtures over silver catalysts: theoretical insights into the role of the particle size. Physical Chemistry Chemical Physics, 2014, 16, 26600-26612.	2.8	18
13	Ketonic Decarboxylation Reaction Mechanism: A Combined Experimental and DFT Study. ChemSusChem, 2013, 6, 141-151.	6.8	121
14	Reconstruction of the carbon sp²network in graphene oxide by low-temperature reaction with CO. Journal of Materials Chemistry, 2012, 22, 51-56.	6.7	26
15	Aerobic epoxidation of propene over silver (111) and (100) facet catalysts. Journal of Catalysis, 2012, 292, 138-147.	6.2	56
16	Propene Epoxidation with H₂/H₂O/O₂ Mixtures Over Gold Atoms Supported on Defective Graphene: A Theoretical Study. Journal of Physical Chemistry C, 2012, 116, 19355-19362.	3.1	26
17	Combined Experimental and Theoretical Investigations of Heterogeneous Dual Cation Sites in Cu,M-FER Zeolites. Journal of Physical Chemistry C, 2011, 115, 13312-13321.	3.1	20
18	Theoretical investigation of gold clusters supported on graphene sheets. New Journal of Chemistry, 2011, 35, 2153.	2.8	31

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19	Combined volumetric, infrared spectroscopic and theoretical investigation of CO2 adsorption on Na-A zeolite. Microporous and Mesoporous Materials, 2011, 146, 97-105.	4.4	75
20	Periodic DFT investigation of the effect of aluminium content on the properties of the acid zeolite H-FER. Physical Chemistry Chemical Physics, 2010, 12, 1497.	2.8	49
21	Experimental and theoretical determination of adsorption heats of CO2 over alkali metal exchanged ferrierites with different Si/Al ratio. Physical Chemistry Chemical Physics, 2010, 12, 6413.	2.8	86
22	Computational and Variableâ€Temperature Infrared Spectroscopic Studies on Carbon Monoxide Adsorption on Zeolite Caâ€A. ChemPhysChem, 2009, 10, 1058-1065.	2.1	14
23	Hydrogen adsorption on the zeolite Ca-A: DFT and FT-IR investigation. Chemical Physics Letters, 2009, 477, 139-143.	2.6	40
24	Correlation Between Catalytic Activity and Metal Cation Coordination: NO Decomposition Over Cu/Zeolites. ChemCatChem, 2009, 1, 449-453.	3.7	20
25	Adsorption of CO₂ on Sodium-Exchanged Ferrierites: The Bridged CO₂ Complexes Formed between Two Extraframework Cations. Journal of Physical Chemistry C, 2009, 113, 2928-2935.	3.1	75
26	Combined DFT/CC and IR spectroscopic studies on carbon dioxide adsorption on the zeolite H-FER. Energy and Environmental Science, 2009, 2, 1187.	30.8	75
27	Theoretical investigation of dinitrosyl complexes in Cu-zeolites as intermediates in deNOx process. Physical Chemistry Chemical Physics, 2009, 11, 1447.	2.8	29
28	Computational and Fourier Transform Infrared Spectroscopic Studies on Carbon Monoxide Adsorption on the Zeolites Na-ZSM-5 and K-ZSM-5:â€‰ Evidence of Dual-Cation Sites. Journal of Physical Chemistry C, 2008, 112, 4658-4666.	3.1	63
29	Evidence of heterogeneous dual cation sites in zeolites by combined IR and DFT investigation. Studies in Surface Science and Catalysis, 2008, , 1005-1008.	1.5	8
30	Computational Study of Location and Role of Fluoride in Zeolite Structures. Journal of Physical Chemistry B, 2006, 110, 23951-23961.	2.6	34
31	Computational Study of19F NMR Spectra of Double Four Ring-Containing Si/Ge-Zeolites. ChemPhysChem, 2006, 7, 1092-1099.	2.1	46
32	An attempt to predict and rationalize relative stabilities and preferential germanium location in Si/Ge zeolites. Microporous and Mesoporous Materials, 2005, 82, 159-163.	4.4	38
33	Pentacoordinated germanium in AST zeolite synthesised in fluoride media. A 19F NMR validated computational study. Chemical Communications, 2005, , 2357.	4.1	22
34	Effect of the Germanium Incorporation in the Synthesis of EU-1, ITQ-13, ITQ-22, and ITQ-24 Zeolites. Journal of Physical Chemistry B, 2004, 108, 8830-8835.	2.6	71