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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	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
2	Functional materials discovery using energyâ€“structureâ€“function maps. Nature, 2017, 543, 657-664.	27.8	348
3	Near-Ideal Xylene Selectivity in Adaptive Molecular Pillar[n]arene Crystals. Journal of the American Chemical Society, 2018, 140, 6921-6930.	13.7	191
4	Reticular synthesis of porous molecular 1D nanotubes and 3D networks. Nature Chemistry, 2017, 9, 17-25.	13.6	122
5	Ketonic Decarboxylation Reaction Mechanism: A Combined Experimental and DFT Study. ChemSusChem, 2013, 6, 141-151.	6.8	121
6	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
7	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
8	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
9	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
10	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
11	Computationally-Guided Synthetic Control over Pore Size in Isostructural Porous Organic Cages. ACS Central Science, 2017, 3, 734-742.	11.3	68
12	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
13	Aerobic epoxidation of propene over silver (111) and (100) facet catalysts. Journal of Catalysis, 2012, 292, 138-147.	6.2	56
14	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
15	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
16	Computational Study of19F NMR Spectra of Double Four Ring-Containing Si/Ge-Zeolites. ChemPhysChem, 2006, 7, 1092-1099.	2.1	46
17	Photocatalytic proton reduction by a computationally identified, molecular hydrogen-bonded framework. Journal of Materials Chemistry A, 2020, 8, 7158-7170.	10.3	45
18	Hydrogen adsorption on the zeolite Ca-A: DFT and FT-IR investigation. Chemical Physics Letters, 2009, 477, 139-143.	2.6	40

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19	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
20	Computational Study of Location and Role of Fluoride in Zeolite Structures. Journal of Physical Chemistry B, 2006, 110, 23951-23961.	2.6	34
21	Theoretical investigation of gold clusters supported on graphene sheets. New Journal of Chemistry, 2011, 35, 2153.	2.8	31
22	Theoretical investigation of dinitrosyl complexes in Cu-zeolites as intermediates in deNOx process. Physical Chemistry Chemical Physics, 2009, 11, 1447.	2.8	29
23	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
24	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
25	From Concept to Crystals via Prediction: Multiâ€Component Organic Cage Pots by Social Selfâ€Sorting. Angewandte Chemie, 2019, 131, 16421-16427.	2.0	23
26	Pentacoordinated germanium in AST zeolite synthesised in fluoride media. A 19F NMR validated computational study. Chemical Communications, 2005, , 2357.	4.1	22
27	Correlation Between Catalytic Activity and Metal Cation Coordination: NO Decomposition Over Cu/Zeolites. ChemCatChem, 2009, 1, 449-453.	3.7	20
28	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
29	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
30	Computational and Variableâ€Temperature Infrared Spectroscopic Studies on Carbon Monoxide Adsorption on Zeolite Caâ€A. ChemPhysChem, 2009, 10, 1058-1065.	2.1	14
31	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
32	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
33	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
34	Applications of crystal structure prediction â€“ organic molecular structures: general discussion. Faraday Discussions, 2018, 211, 493-539.	3.2	8