Mercedes Boronat

List of Publications by Year
in descending order

60 papers	4,887 citations	100601 38 h-index	145109 60 g-index
60 all docs	60 docs citations	60 times ranked	6591 citing authors

#	Article	IF	Citations
1	The 2D or 3D morphology of sub-nanometer Cu₅ and Cu₈ clusters changes the mechanism of CO oxidation. Physical Chemistry Chemical Physics, 2022, 24, 4504-4514.	1.3	3
2	Direct assessment of confinement effect in zeolite-encapsulated subnanometric metal species. Nature Communications, 2022, 13, 821.	5.8	30
3	A Career in Catalysis: Avelino Corma. ACS Catalysis, 2022, 12, 7054-7123.	5.5	14
4	The Limits of the Confinement Effect Associated to Cage Topology on the Control of the MTO Selectivity. ChemCatChem, 2021, 13, 1578-1586.	1.8	18
5	Hydrogenation of substituted nitroaromatics on non-noble metal catalysts: mechanistic insights to improve selectivity. Faraday Discussions, 2021, 229, 297-317.	1.6	7
6	Tailoring Lewis/BrÃ¸nsted acid properties of MOF nodes <i>via</i> hydrothermal and solvothermal synthesis: simple approach with exceptional catalytic implications. Chemical Science, 2021, 12, 10106-10115.	3.7	40
7	Advanced approaches: general discussion. Faraday Discussions, 2021, 229, 378-421.	1.6	1
8	Soluble/MOF-Supported Palladium Single Atoms Catalyze the Ligand-, Additive-, and Solvent-Free Aerobic Oxidation of Benzyl Alcohols to Benzoic Acids. Journal of the American Chemical Society, 2021, 143, 2581-2592.	6.6	74
9	Regioirregular and catalytic Mizorokiâ€“Heck reactions. Nature Catalysis, 2021, 4, 293-303.	16.1	42
10	<i>In-Situ</i>-Generated Active Hf-hydride in Zeolites for the Tandem N-Alkylation of Amines with Benzyl Alcohol. ACS Catalysis, 2021, 11, 8049-8061.	5.5	29
11	Design and Synthesis of the Active Site Environment in Zeolite Catalysts for Selectively Manipulating Mechanistic Pathways. Journal of the American Chemical Society, 2021, 143, 10718-10726.	6.6	23
12	Combined Spectroscopic and Computational Study of Nitrobenzene Activation on Non-Noble Metals-Based Mono- and Bimetallic Catalysts. Nanomaterials, 2021, 11, 2037.	1.9	5
13	Mobility and Reactivity of Cu⁺ Species in Cu-CHA Catalysts under NH₃-SCR-NOx Reaction Conditions: Insights from AIMD Simulations. Jacs Au, 2021, 1, 1778-1787.	3.6	27
14	Unraveling the Reaction Mechanism and Active Sites of Metalâ€“Organic Frameworks for Glucose Transformations in Water: Experimental and Theoretical Studies. ACS Sustainable Chemistry and Engineering, 2020, 8, 16143-16155.	3.2	19
15	Production of aromatics from biomass by computer-aided selection of the zeolite catalyst. Green Chemistry, 2020, 22, 5123-5131.	4.6	25
16	Theoretical and Spectroscopic Evidence of the Dynamic Nature of Copper Active Sites in Cu-CHA Catalysts under Selective Catalytic Reduction (NH₃â€“SCRâ€“NO_{<i>x</i>}) Conditions. Journal of Physical Chemistry Letters, 2020, 11, 10060-10066.	2.1	27
17	The Crucial Role of Cluster Morphology on the Epoxidation of Propene Catalyzed by Cu₅: A DFT Study. Journal of Physical Chemistry C, 2020, 124, 21549-21558.	1.5	12
18	Selective active site placement in Lewis acid zeolites and implications for catalysis of oxygenated compounds. Chemical Science, 2020, 11, 10225-10235.	3.7	23

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19	Impact of Zeolite Framework Composition and Flexibility on Methanolâ€Toâ€Olefins Selectivity: Confinement or Diffusion?. Angewandte Chemie, 2020, 132, 19876-19883.	1.6	11
20	Organicâ€Free Synthesis of Zeolite Y with High Si/Al Ratios: Combined Strategy of In Situ Hydroxyl Radical Assistance and Postâ€Synthesis Treatment. Angewandte Chemie, 2020, 132, 17378-17381.	1.6	14
21	Organicâ€Free Synthesis of Zeolite Y with High Si/Al Ratios: Combined Strategy of In Situ Hydroxyl Radical Assistance and Postâ€Synthesis Treatment. Angewandte Chemie - International Edition, 2020, 59, 17225-17228.	7.2	47
22	Impact of Zeolite Framework Composition and Flexibility on Methanolâ€Toâ€Olefins Selectivity: Confinement or Diffusion?. Angewandte Chemie - International Edition, 2020, 59, 19708-19715.	7.2	52
23	Control of the Reaction Mechanism of Alkylaromatics Transalkylation by Means of Molecular Confinement Effects Associated to Zeolite Channel Architecture. ACS Catalysis, 2019, 9, 5935-5946.	5.5	29
24	Spectroscopic Evidence and Density Functional Theory (DFT) Analysis of Low-Temperature Oxidation of Cu⁺ to Cu²⁺NO_{<i>x</i>} in Cu-CHA Catalysts: Implications for the SCR-NO_{<i>x</i>} Reaction Mechanism. ACS Catalysis, 2019, 9, 2725-2738.	5.5	55
25	Low-Temperature Catalytic NO Reduction with CO by Subnanometric Pt Clusters. ACS Catalysis, 2019, 9, 11530-11541.	5.5	70
26	Chemical and Structural Parameter Connecting Cavity Architecture, Confined Hydrocarbon Pool Species, and MTO Product Selectivity in Small-Pore Cage-Based Zeolites. ACS Catalysis, 2019, 9, 11542-11551.	5.5	51
27	What Is Measured When Measuring Acidity in Zeolites with Probe Molecules?. ACS Catalysis, 2019, 9, 1539-1548.	5.5	111
28	Base-Controlled Heck, Suzuki, and Sonogashira Reactions Catalyzed by Ligand-Free Platinum or Palladium Single Atom and Sub-Nanometer Clusters. Journal of the American Chemical Society, 2019, 141, 1928-1940.	6.6	107
29	Sub nanometer clusters in catalysis. Journal of Physics Condensed Matter, 2019, 31, 013002.	0.7	23
30	Modeling of EPR Parameters for Cu(II): Application to the Selective Reduction of NOx Catalyzed by Cu-Zeolites. Topics in Catalysis, 2018, 61, 810-832.	1.3	26
31	Synthesis of Densely Packaged, Ultrasmall Pt⁰₂ Clusters within a Thioetherâ€Functionalized MOF: Catalytic Activity in Industrial Reactions at Low Temperature. Angewandte Chemie - International Edition, 2018, 57, 6186-6191.	7.2	115
32	Radical-Facilitated Green Synthesis of Highly Ordered Mesoporous Silica Materials. Journal of the American Chemical Society, 2018, 140, 4770-4773.	6.6	91
33	Confined Pt₁¹⁺ Water Clusters in a MOF Catalyze the Lowâ€Temperature Waterâ€"Gas Shift Reaction with both CO₂ Oxygen Atoms Coming from Water. Angewandte Chemie - International Edition, 2018, 57, 17094-17099.	7.2	54
34	A new molecular pathway allows the chemoselective reduction of nitroaromatics on non-noble metal catalysts. Journal of Catalysis, 2018, 364, 19-30.	3.1	57
35	Making Nanosized CHA Zeolites with Controlled Al Distribution for Optimizing Methanolâ€toâ€Olefin Performance. Chemistry - A European Journal, 2018, 24, 14631-14635.	1.7	57
36	Synthesis of reactionâ€adapted zeolites as methanol-to-olefins catalysts with mimics of reaction intermediates as organic structureâ€directing agents. Nature Catalysis, 2018, 1, 547-554.	16.1	111

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37	Selective Introduction of Acid Sites in Different Confined Positions in ZSM-5 and Its Catalytic Implications. ACS Catalysis, 2018, 8, 7688-7697.	5.5	139
38	â€œAb initioâ€•synthesis of zeolites for preestablished catalytic reactions. Science, 2017, 355, 1051-1054.	6.0	204
39	Enhanced Stability of Cu Clusters of Low Atomicity against Oxidation. Effect on the Catalytic Redox Process. ACS Catalysis, 2017, 7, 3560-3568.	5.5	58
40	Structureâ€“reactivity relationship in isolated Zr sites present in Zr-zeolite and ZrO₂ for the Meerweinâ€“Ponndorfâ€“Verley reaction. Catalysis Science and Technology, 2017, 7, 2865-2873.	2.1	52
41	The MOF-driven synthesis of supported palladium clusters with catalytic activity for carbene-mediated chemistry. Nature Materials, 2017, 16, 760-766.	13.3	230
42	Accelerated crystallization of zeolites via hydroxyl free radicals. Science, 2016, 351, 1188-1191.	6.0	297
43	Ammonia-Containing Species Formed in Cu-Chabazite As Per In Situ EPR, Solid-State NMR, and DFT Calculations. Journal of Physical Chemistry Letters, 2015, 6, 1011-1017.	2.1	72
44	Factors Controlling the Acidity of Zeolites. Catalysis Letters, 2015, 145, 162-172.	1.4	65
45	Trends in the Reactivity of Molecular O₂ with Copper Clusters: Influence of Size and Shape. Journal of Physical Chemistry C, 2015, 119, 19832-19846.	1.5	63
46	Making Câ€“C Bonds with Gold Catalysts: A Theoretical Study of the Influence of Gold Particle Size on the Dissociation of the Câ€“X Bond in Aryl Halides. Journal of Physical Chemistry C, 2014, 118, 9018-9029.	1.5	11
47	Theoretical and Experimental Insights into the Origin of the Catalytic Activity of Subnanometric Gold Clusters: Attempts to Predict Reactivity with Clusters and Nanoparticles of Gold. Accounts of Chemical Research, 2014, 47, 834-844.	7.6	210
48	Exceptional oxidation activity with size-controlled supported gold clusters of low atomicity. Nature Chemistry, 2013, 5, 775-781.	6.6	394
49	Making Câ€“C Bonds with Gold: Identification of Selective Gold Sites for Homo- and Cross-Coupling Reactions between Iodobenzene and Alkynes. Journal of Physical Chemistry C, 2012, 116, 24855-24867.	1.5	65
50	Aerobic epoxidation of propene over silver (111) and (100) facet catalysts. Journal of Catalysis, 2012, 292, 138-147.	3.1	56
51	Synthesis and Stabilization of Subnanometric Gold Oxide Nanoparticles on Multiwalled Carbon Nanotubes and Their Catalytic Activity. Journal of the American Chemical Society, 2011, 133, 10251-10261.	6.6	87
52	Gold catalyzes the Sonogashira coupling reaction without the requirement of palladium impurities. Chemical Communications, 2011, 47, 1446-1448.	2.2	163
53	Tuning the Behavior of Au and Pt Catalysts for the Chemoselective Hydrogenation of Nitroaromatic Compounds. Topics in Catalysis, 2011, 54, 439-446.	1.3	82
54	Oxygen activation on gold nanoparticles: separating the influence of particle size, particle shape and support interaction. Dalton Transactions, 2010, 39, 8538.	1.6	134

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55	Origin of the Different Activity and Selectivity toward Hydrogenation of Single Metal Au and Pt on TiO₂ and Bimetallic Auâˆ’Pt/TiO₂ Catalysts. Langmuir, 2010, 26, 16607-16614.	1.6	77
56	Enzyme-like Specificity in Zeolites: A Unique Site Position in Mordenite for Selective Carbonylation of Methanol and Dimethyl Ether with CO. Journal of the American Chemical Society, 2008, 130, 16316-16323.	6.6	266
57	Peculiarities of Sn-Beta and potential industrial applications. Catalysis Today, 2007, 121, 39-44.	2.2	58
58	Mechanism of the Meerweinâˆ’Ponndorfâˆ’Verleyâˆ’Oppenauer (MPVO) Redox Equilibrium on Snâˆ’ and Zrâˆ’Beta Zeolite Catalysts. Journal of Physical Chemistry B, 2006, 110, 21168-21174.	1.2	216
59	Predicting the Activity of Single Isolated Lewis Acid Sites in Solid Catalysts. Chemistry - A European Journal, 2006, 12, 7067-7077.	1.7	108
60	Determination of the catalytically active oxidation Lewis acid sites in Sn-beta zeolites, and their optimisation by the combination of theoretical and experimental studies. Journal of Catalysis, 2005, 234, 111-118.	3.1	280