CÃ©line Chizallet

List of Publications by Year
in descending order

89 papers	4,841 citations	87886 38 h-index	95259 68 g-index
95 all docs	95 docs citations	95 times ranked	5713 citing authors

#	Article	IF	Citations
1	Achievements and Expectations in the Field of Computational Heterogeneous Catalysis in an Innovation Context. Topics in Catalysis, 2022, 65, 69-81.	2.8	16
2	Revisiting Î³-alumina surface models through the topotactic transformation of boehmite surfaces. Journal of Catalysis, 2022, 405, 140-151.	6.2	14
3	Multiscale Modeling as a Tool for the Prediction of Catalytic Performances: The Case of n-Heptane Hydroconversion in a Large-Pore Zeolite. ACS Catalysis, 2022, 12, 1068-1081.	11.2	21
4	Evidence for H₂-Induced Ductility in a Pt/Al₂O₃ Catalyst. ACS Catalysis, 2022, 12, 5979-5989.	11.2	9
5	Evaluating acid and metallic site proximity in Pt/Î³-Al₂O₃â€“Cl bifunctional catalysts through an atomic scale geometrical model. Nanoscale, 2022, 14, 8753-8765.	5.6	6
6	Multiscale Visualization and Quantification of the Effect of Binders on the Acidity of Shaped Zeolites. ACS Catalysis, 2022, 12, 6794-6808.	11.2	9
7	Surface orientation dependent interaction of cobalt (II) precursors with alpha-alumina. Journal of Catalysis, 2021, 394, 157-166.	6.2	2
8	Ethylcyclohexane Hydroconversion in EUâ€1 Zeolite: DFTâ€based Microkinetic Modeling Reveals the Nature of the Kinetically Relevant Intermediates. ChemCatChem, 2021, 13, 3434-3442.	3.7	2
9	Spectroscopic Expression of the External Surface Sites of H-ZSM-5. Journal of Physical Chemistry C, 2021, 125, 2163-2181.	3.1	34
10	Thermokinetic and Spectroscopic Mapping of Carbon Monoxide Adsorption on Highly Dispersed Pt/Î³-Al₂O₃. ACS Catalysis, 2021, 11, 13280-13293.	11.2	17
11	IZM-7: A new stable aluminosilicogermanate with a promising catalytic activity. Journal of Catalysis, 2021, , .	6.2	1
12	Dynamic Features of Transition States for Î²â€Scission Reactions of Alkenes over Acid Zeolites Revealed by AIMD Simulations. Angewandte Chemie, 2020, 132, 19100-19104.	2.0	9
13	Dynamic Features of Transition States for Î²â€Scission Reactions of Alkenes over Acid Zeolites Revealed by AIMD Simulations. Angewandte Chemie - International Edition, 2020, 59, 18938-18942.	13.8	20
14	Atomic Scale Insight into the Formation, Size, and Location of Platinum Nanoparticles Supported on Î³-Alumina. ACS Catalysis, 2020, 10, 4193-4204.	11.2	30
15	Ab initio investigation of the relative stability of silicogermanates and their (Alumino)Silicates counterparts. Microporous and Mesoporous Materials, 2020, 306, 110425.	4.4	3
16	Environment, Stability and Acidity of External Surface Sites of Silicalite-1 and ZSM-5 Micro and Nano Slabs, Sheets, and Crystals. ACS Catalysis, 2020, 10, 3297-3312.	11.2	32
17	Toward the Atomic Scale Simulation of Intricate Acidic Aluminosilicate Catalysts. ACS Catalysis, 2020, 10, 5579-5601.	11.2	49
18	Interplay of the adsorption of light and heavy paraffins in hydroisomerization over H-beta zeolite. Catalysis Science and Technology, 2019, 9, 5368-5382.	4.1	12

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19	Competition of Secondary versus Tertiary Carbenium Routes for the Type B Isomerization of Alkenes over Acid Zeolites Quantified by Ab Initio Molecular Dynamics Simulations. ACS Catalysis, 2019, 9, 9813-9828.	11.2	35
20	Beyond Î³-Al2O3 crystallite surfaces: The hidden features of edges revealed by solid-state 1H NMR and DFT calculations. Journal of Catalysis, 2019, 378, 140-143.	6.2	36
21	Location of the Active Sites for Ethylcyclohexane Hydroisomerization by Ring Contraction and Expansion in the EUO Zeolitic Framework. ACS Catalysis, 2019, 9, 1692-1704.	11.2	14
22	Atomistic Models for Highlyâ€Dispersed PtSn/Î³â€Al₂O₃ Catalysts: Ductility and Dilution Affect the Affinity for Hydrogen. ChemCatChem, 2019, 11, 3941-3951.	3.7	19
23	On the origin of the difference between type A and type B skeletal isomerization of alkenes catalyzed by zeolites: The crucial input of ab initio molecular dynamics. Journal of Catalysis, 2019, 373, 361-373.	6.2	38
24	Atmosphere-dependent stability and mobility of catalytic Pt single atoms and clusters on Î³-Al₂O₃. Nanoscale, 2019, 11, 6897-6904.	5.6	66
25	Dehydrogenation mechanisms of methyl-cyclohexane on Î³-Al2O3 supported Pt13: Impact of cluster ductility. Journal of Catalysis, 2019, 370, 118-129.	6.2	47
26	Multiscale Approach to the Dissociative Adsorption of Oxygen on a Highly Dispersed Platinum Supported on Î³-Al₂O₃. Journal of Physical Chemistry C, 2018, 122, 26974-26986.	3.1	14
27	Modeling Ammonia and Water Co-Adsorption in CuI-SSZ-13 Zeolite Using DFT Calculations. Industrial & Engineering Chemistry Research, 2018, 57, 15982-15990.	3.7	7
28	Metal/Acid Bifunctional Catalysis and Intimacy Criterion for Ethylcyclohexane Hydroconversion: When Proximity Does Not Matter. ACS Catalysis, 2018, 8, 6035-6046.	11.2	51
29	Biomass-mediated ZSM-5 zeolite synthesis: when self-assembly allows to cross the Si/Al lower limit. Chemical Science, 2018, 9, 6532-6539.	7.4	26
30	Copper Coordination to Water and Ammonia in Cu^{II}-Exchanged SSZ-13: Atomistic Insights from DFT Calculations and in Situ XAS Experiments. Journal of Physical Chemistry C, 2018, 122, 16741-16755.	3.1	31
31	GECat 2015. Comptes Rendus Chimie, 2017, 20, 5-6.	0.5	1
32	Abâ€...Initio Simulation of the Acid Sites at the External Surface of Zeolite Beta. ChemCatChem, 2017, 9, 2176-2185.	3.7	32
33	Isopropanol Dehydration on Amorphous Silicaâ€“Alumina: Synergy of BrÃ¸nsted and Lewis Acidities at Pseudoâ€Bridging Silanols. Angewandte Chemie - International Edition, 2017, 56, 230-234.	13.8	47
34	Isopropanol Dehydration on Amorphous Silica-Alumina: Synergy of BrÃ¸nsted and Lewis Acidities at Pseudo-Bridging Silanols. Angewandte Chemie, 2017, 129, 236-240.	2.0	10
35	The Pivotal Role of Catalysis in France: Selected Examples of Recent Advances and Future Prospects.. ChemCatChem, 2017, 9, 2029-2064.	3.7	2
36	Thermodynamic Characterization of the Hydroxyl Group on the Î³-Alumina Surface by the Energy Distribution Function. Journal of Physical Chemistry C, 2017, 121, 16770-16782.	3.1	33

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37	The French Conference on Catalysisâ€"FCCatâ€...1. ChemCatChem, 2017, 9, 2024-2026.	3.7	0
38	Catalytic Reforming: Methodology and Process Development for a Constant Optimisation and Performance Enhancement. Oil and Gas Science and Technology, 2016, 71, 41.	1.4	14
39	Dealumination mechanisms of zeolites and extra-framework aluminum confinement. Journal of Catalysis, 2016, 339, 242-255.	6.2	149
40	French Catalysis and Much More at FCCatâ€...1. ChemCatChem, 2016, 8, 3170-3174.	3.7	0
41	Influence of Coadsorbed Water and Alcohol Molecules on Isopropyl Alcohol Dehydration on Î³-Alumina: Multiscale Modeling of Experimental Kinetic Profiles. ACS Catalysis, 2016, 6, 1905-1920.	11.2	43
42	Tuning the Metalâ€"Support Interaction by Structural Recognition of Cobaltâ€Based Catalyst Precursors. Angewandte Chemie - International Edition, 2015, 54, 6824-6827.	13.8	30
43	Revisiting carbenium chemistry on amorphous silica-alumina: Unraveling their milder acidity as compared to zeolites. Journal of Catalysis, 2015, 325, 35-47.	6.2	45
44	Mechanistic Investigation of Isopropanol Conversion on Alumina Catalysts: Location of Active Sites for Alkene/Ether Production. ACS Catalysis, 2015, 5, 4423-4437.	11.2	92
45	Atomic Description of the Interface between Silica and Alumina in Aluminosilicates through Dynamic Nuclear Polarization Surface-Enhanced NMR Spectroscopy and First-Principles Calculations. Journal of the American Chemical Society, 2015, 137, 10710-10719.	13.7	129
46	Regioselectivity of Alâ€"O Bond Hydrolysis during Zeolites Dealumination Unified by BrÃ¸nstedâ€"Evansâ€"Polanyi Relationship. ACS Catalysis, 2015, 5, 11-15.	11.2	73
47	Challenges on molecular aspects of dealumination and desilication of zeolites. Microporous and Mesoporous Materials, 2014, 191, 82-96.	4.4	240
48	Density functional theory simulations of complex catalytic materials in reactive environments: beyond the ideal surface at low coverage. Catalysis Science and Technology, 2014, 4, 2797-2813.	4.1	57
49	Monitoring Morphology and Hydrogen Coverage of Nanometric Pt/Î³â€Al₂O₃ Particles by Inâ€...Situ HERFDâ€"XANES and Quantum Simulations. Angewandte Chemie - International Edition, 2014, 53, 12426-12429.	13.8	47
50	From Î³-alumina to supported platinum nanoclusters in reforming conditions: 10years of DFT modeling and beyond. Journal of Catalysis, 2013, 308, 328-340.	6.2	73
51	Role of oxygen vacancies in the basicity of ZnO: From the model methylbutynol conversion to the ethanol transformation application. Applied Catalysis A: General, 2013, 453, 121-129.	4.3	49
52	Origins of the deactivation process in the conversion of methylbutynol on zinc oxide monitored by operando DRIFTS. Catalysis Today, 2013, 205, 67-75.	4.4	18
53	Multiscale Modeling of Barium Sulfate Formation from BaO. Industrial & Engineering Chemistry Research, 2013, 52, 9086-9098.	3.7	3
54	Sulfur Deactivation of NO_xStorage Catalysts: A Multiscale Modeling Approach. Oil and Gas Science and Technology, 2013, 68, 995-1005.	1.4	4

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55	Comment on â€œElectronic properties and charge transfer phenomena in Pt nanoparticles on Î³-Al2O3: size, shape, support, and adsorbate effectsâ€•by F. Behafarid et al., Phys. Chem. Chem. Phys., 2012, 14, 11766â€“11779. Physical Chemistry Chemical Physics, 2012, 14, 16773.	2.8	8
56	Adsorption and Separation of Xylene Isomers: CPO-27-Ni vs HKUST-1 vs NaY. Journal of Physical Chemistry C, 2012, 116, 21844-21855.	3.1	72
57	ZnO Oxygen Vacancies Formation and Filling Followed by in Situ Photoluminescence and in Situ EPR. Journal of Physical Chemistry C, 2012, 116, 21297-21307.	3.1	164
58	The Origin of the Activity of Amineâ€Functionalized Metalâ€“Organic Frameworks in the Catalytic Synthesis of Cyclic Carbonates from Epoxide and CO₂. ChemCatChem, 2012, 4, 1725-1728.	3.7	91
59	Effect of Indium Doping of Î³-Alumina on the Stabilization of PtSn Alloyed Clusters Prepared by Surface Organostannic Chemistry. Journal of Physical Chemistry C, 2012, 116, 10073-10083.	3.1	25
60	Comparison of the Behavior of Metalâ€“Organic Frameworks and Zeolites for Hydrocarbon Separations. Journal of the American Chemical Society, 2012, 134, 8115-8126.	13.7	253
61	Platinum Nanoclusters Stabilized on Î³-Alumina by Chlorine Used As a Capping Surface Ligand: A Density Functional Theory Study. ACS Catalysis, 2012, 2, 1346-1357.	11.2	77
62	CO adsorption on amorphous silicaâ€“alumina: electrostatic or BrÃ¸nsted acidity probe?. Chemical Communications, 2012, 48, 4076.	4.1	35
63	A Molecular Approach for Unraveling Surface Phase Transitions: Sulfation of BaO as a Model NO_x Trap. Chemistry - A European Journal, 2012, 18, 10511-10514.	3.3	3
64	Experimental and Computational Study of Functionality Impact on Sodaliteâ€“Zeolitic Imidazolate Frameworks for CO₂Separation. Journal of Physical Chemistry C, 2011, 115, 16425-16432.	3.1	128
65	Thermodynamic Stability of Buta-1,3-diene and But-1-ene on Pd(111) and (100) Surfaces under H₂ Pressure: A DFT Study. Journal of Physical Chemistry C, 2011, 115, 12135-12149.	3.1	40
66	BrÃ¸nsted acidity of amorphous silicaâ€“alumina: The molecular rules of proton transfer. Journal of Catalysis, 2011, 284, 215-229.	6.2	96
67	H₂â€Induced Reconstruction of Supported Pt Clusters: Metalâ€“Support Interaction versus Surface Hydride. ChemCatChem, 2011, 3, 200-207.	3.7	152
68	Investigation of Acid Centers in MILâ€53(Al, Ga) for BrÃ¸nstedâ€Type Catalysis: Inâ€…Situ FTIR and Abâ€…Initio Molecular Modeling. ChemCatChem, 2010, 2, 1235-1238.	3.7	72
69	Modulation of catalyst particle structure upon support hydroxylation: Ab initio insights into Pd13 and Pt13/Î³-Al2O3. Journal of Catalysis, 2010, 274, 99-110.	6.2	137
70	Acidity of Amorphous Silicaâ€“Alumina: From Coordination Promotion of Lewis Sites to Proton Transfer. ChemPhysChem, 2010, 11, 105-108.	2.1	56
71	Basic reactivity of CaO: investigating active sites under operating conditions. Physical Chemistry Chemical Physics, 2010, 12, 14740.	2.8	27
72	External Surface of Zeolite Imidazolate Frameworks Viewed Ab Initio: Multifunctionality at the Organicâ^'Inorganic Interface. Journal of Physical Chemistry Letters, 2010, 1, 349-353.	4.6	82

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73	Catalysis of Transesterification by a Nonfunctionalized Metalâ"Organic Framework: Acido-Basicity at the External Surface of ZIF-8 Probed by FTIR and ab Initio Calculations. Journal of the American Chemical Society, 2010, 132, 12365-12377.	13.7	503
74	Structural, energetic, and electronic trends in low-dimensional late-transition-metal systems. Physical Review B, 2009, 79, .	3.2	31
75	Identification of the OH groups responsible for kinetic basicity on MgO surfaces by 1H MAS NMR. Journal of Catalysis, 2009, 268, 175-179.	6.2	36
76	Pseudoâ€Bridging Silanols as Versatile BrÃ¸nsted Acid Sites of Amorphous Aluminosilicate Surfaces. Angewandte Chemie - International Edition, 2009, 48, 2891-2893.	13.8	109
77	Insights into the Geometry, Stability and Vibrational Properties of OH Groups on Î³-Al2O3, TiO2-Anatase and MgO from DFT Calculations. Topics in Catalysis, 2009, 52, 1005-1016.	2.8	34
78	Growth of boehmite particles in the presence of xylitol: morphology oriented by the nest effect of hydrogen bonding. Physical Chemistry Chemical Physics, 2009, 11, 11310.	2.8	53
79	Assignment of Photoluminescence Spectra of MgO Powders: TD-DFT Cluster Calculations Combined to Experiments. Part I: Structure Effects on Dehydroxylated Surfaces. Journal of Physical Chemistry C, 2008, 112, 16629-16637.	3.1	40
80	Assignment of Photoluminescence Spectra of MgO Powders: TD-DFT Cluster Calculations Combined to Experiments. Part II. Hydroxylation Effects. Journal of Physical Chemistry C, 2008, 112, 19710-19717.	3.1	25
81	Infrared Characterization of Hydroxyl Groups on MgO:â€‰ A Periodic and Cluster Density Functional Theory Study. Journal of the American Chemical Society, 2007, 129, 6442-6452.	13.7	125
82	Study of the Structure of OH Groups on MgO by 1D and 2D ¹H MAS NMR Combined with DFT Cluster Calculations. Journal of Physical Chemistry C, 2007, 111, 18279-18287.	3.1	38
83	Revisiting Acido-basicity of the MgO Surface by Periodic Density Functional Theory Calculations:Â Role of Surface Topology and Ion Coordination on Water Dissociation. Journal of Physical Chemistry B, 2006, 110, 15878-15886.	2.6	125
84	Role of Hydroxyl Groups in the Basic Reactivity of MgO: a Theoretical and Experimental Study. Oil and Gas Science and Technology, 2006, 61, 479-488.	1.4	31
85	Thermodynamic brÃ¸nsted basicity of clean MgO surfaces determined by their deprotonation ability: Role of Mg2+â€"O2â" pairs. Catalysis Today, 2006, 116, 196-205.	4.4	54
86	1H MAS NMR study of the coordination of hydroxyl groups generated upon adsorption of H2O and CD3OH on clean MgO surfaces. Applied Catalysis A: General, 2006, 307, 239-244.	4.3	16
87	Kinetic Model of Energy Transfer Processes Between Low-Coordinated Ions on MgO by Photoluminescence Decay Measurements. ChemPhysChem, 2006, 7, 904-911.	2.1	16
88	Water on extended and point defects at MgO surfaces. Journal of Chemical Physics, 2006, 125, 054702.	3.0	48
89	A spectroscopy and catalysis study of the nature of active sites of MgO catalysts: Thermodynamic BrÃ¸nsted basicity versus reactivity of basic sites. Journal of Catalysis, 2005, 235, 413-422.	6.2	127