Pascal Raybaud

List of Publications by Year
in descending order

133	10,632	28274	32842
papers	citations	55 h-index	100 g-index

140	140	140	8526
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Use of DFT to achieve a rational understanding of acid?basic properties of ?-alumina surfaces. Journal of Catalysis, 2004, 226, 54-68.	6.2	880
2	Theoretical Study of the Dehydration Process of Boehmite to Î³-Alumina. Journal of Physical Chemistry B, 2001, 105, 5121-5130.	2.6	435
3	Hydroxyl Groups on Î³-Alumina Surfaces: A DFT Study. Journal of Catalysis, 2002, 211, 1-5.	6.2	364
4	Ab Initio Study of the H2â€“H2S/MoS2 Gasâ€“Solid Interface: The Nature of the Catalytically Active Sites. Journal of Catalysis, 2000, 189, 129-146.	6.2	350
5	Shape and Edge Sites Modifications of MoS2 Catalytic Nanoparticles Induced by Working Conditions: A Theoretical Study. Journal of Catalysis, 2002, 207, 76-87.	6.2	337
6	Structure, Energetics, and Electronic Properties of the Surface of a Promoted MoS2 Catalyst: An ab Initio Local Density Functional Study. Journal of Catalysis, 2000, 190, 128-143.	6.2	321
7	Effects of morphology on surface hydroxyl concentration: a DFT comparison of anataseâ€“TiO2 and Î³-alumina catalytic supports. Journal of Catalysis, 2004, 222, 152-166.	6.2	300
8	Structure and Stability of Aluminum Hydroxides:Â A Theoretical Study. Journal of Physical Chemistry B, 2002, 106, 5155-5162.	2.6	241
9	Challenges on molecular aspects of dealumination and desilication of zeolites. Microporous and Mesoporous Materials, 2014, 191, 82-96.	4.4	240
10	Morphology and Surface Properties of Boehmite (Î³-AlOOH): A Density Functional Theory Study. Journal of Catalysis, 2001, 201, 236-246.	6.2	218
11	Periodic trends in hydrodesulfurization: in support of the Sabatier principle. Applied Catalysis A: General, 2002, 227, 83-96.	4.3	189
12	Optimal promoter edge decoration of CoMoS catalysts: A combined theoretical and experimental study. Catalysis Today, 2008, 130, 149-159.	4.4	184
13	Promoter Sensitive Shapes of Co(Ni)MoS Nanocatalysts in Sulfo-Reductive Conditions. Journal of Catalysis, 2002, 212, 33-38.	6.2	173
14	Kinetic interpretation of catalytic activity patterns based on theoretical chemical descriptors. Journal of Catalysis, 2003, 216, 63-72.	6.2	165
15	Transition metals to sulfur binding energies relationship to catalytic activities in HDS: back to Sabatier with first principle calculations1This work has been undertaken within the â€œGdR Dynamique MolÃ©culaire Quantique AppliquÃ©e Ã la Catalyseâ€, a joint project of Centre National de la Recherche Scientifique, Technische UniversitÃt Wien, and Institut FranÃ§ais du PÃ©trole.1. Catalysis Today, 1999, 50, 629-636.	4.4	152
16	H₂â€induced Reconstruction of Supported Pt Clusters: Metalâ€“Support Interaction versus Surface Hydride. ChemCatChem, 2011, 3, 200-207.	3.7	152
17	Dealumination mechanisms of zeolites and extra-framework aluminum confinement. Journal of Catalysis, 2016, 339, 242-255.	6.2	149
18	Adsorption of Unsaturated Hydrocarbons on Pd(111) and Pt(111): A DFT Study. Journal of Physical Chemistry B, 2003, 107, 12287-12295.	2.6	148

#	Article	IF	Citations
19	Mixed sites and promoter segregation: A DFT study of the manifestation of Le Chatelier's principle for the Co(Ni)MoS active phase in reaction conditions. Catalysis Today, 2008, 130, 160-169.	4.4	147
20	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
21	Understanding and predicting improved sulfide catalysts: Insights from first principles modeling. Applied Catalysis A: General, 2007, 322, 76-91.	4.3	136
22	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
23	Adsorption of Thiophene on the Catalytically Active Surface ofMoS2: AnAb InitioLocal-Density-Functional Study. Physical Review Letters, 1998, 80, 1481-1484.	7.8	128
24	Ab initiodensity functional studies of transition-metal sulphides: I. Crystal structure and cohesive properties. Journal of Physics Condensed Matter, 1997, 9, 11085-11106.	1.8	118
25	Hydrodeoxygenation pathways catalyzed by MoS2 and NiMoS active phases: A DFT study. Journal of Catalysis, 2011, 279, 276-286.	6.2	118
26	The role of the extra-framework cations in the adsorption of CO2 on faujasite Y. Physical Chemistry Chemical Physics, 2010, 12, 13534.	2.8	117
27	Free-energy profiles along reduction pathways of MoS2 M-edge and S-edge by dihydrogen: A first-principles study. Journal of Catalysis, 2011, 280, 178-195.	6.2	117
28	Ab initiodensity functional studies of transition-metal sulphides: II. Electronic structure. Journal of Physics Condensed Matter, 1997, 9, 11107-11140.	1.8	109
29	Hemilabile Ligand Induced Selectivity:â€‰a DFT Study on Ethylene Trimerization Catalyzed by Titanium Complexes. Organometallics, 2003, 22, 3404-3413.	2.3	109
30	Pseudoâ€Bridging Silanols as Versatile BrÃ¸nsted Acid Sites of Amorphous Aluminosilicate Surfaces. Angewandte Chemie - International Edition, 2009, 48, 2891-2893.	13.8	109
31	Structural and electronic properties of the MoS2(101Ì„0) edge-surface. Surface Science, 1998, 407, 237-250.	1.9	108
32	Deoxygenation mechanisms on Ni-promoted MoS2 bulk catalysts: A combined experimental and theoretical study. Journal of Catalysis, 2012, 286, 153-164.	6.2	107
33	A density functional theory comparison of anatase (TiO2)- and Î³-Al2O3-supported MoS2 catalysts. Journal of Catalysis, 2005, 232, 161-178.	6.2	105
34	The Origin of the C7-Hydroconversion Selectivities on Y, Î², ZSM-22, ZSM-23, and EU-1 Zeolites. Journal of Catalysis, 2001, 197, 98-112.	6.2	104
35	Influence of the Hydroxylation of Î³-Al2O3Surfaces on the Stability and Diffusion of Single Pd Atoms:Â A DFT Study. Journal of Physical Chemistry B, 2006, 110, 1759-1767.	2.6	103
36	BrÃ¸nsted acidity of amorphous silicaâ€“alumina: The molecular rules of proton transfer. Journal of Catalysis, 2011, 284, 215-229.	6.2	96

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37	Origin of the Enhanced Visible-Light Absorption in N-Doped Bulk Anatase TiO₂ from First-Principles Calculations. Journal of Physical Chemistry C, 2011, 115, 19394-19404.	3.1	91
38	Edge wetting effects of Î³-Al2O3 and anatase-TiO2 supports by MoS2 and CoMoS active phases: A DFT study. Journal of Catalysis, 2007, 246, 325-343.	6.2	87
39	Tuning the properties of visible-light-responsive tantalum (oxy)nitride photocatalysts by non-stoichiometric compositions: a first-principles viewpoint. Physical Chemistry Chemical Physics, 2014, 16, 20548-20560.	2.8	86
40	Nucleation ofPdn(n=1â€“5)clusters and wetting of Pd particles onÎ³â^'Al2O3surfaces: A density functional theory study. Physical Review B, 2007, 75, .	3.2	84
41	Interplay between molecular adsorption and metalâ€“support interaction for small supported metal clusters: CO and C2H4 adsorption on Pd4/Î³Pd4/Î³-Al2O3. Journal of Catalysis, 2007, 247, 339-355.	6.2	80
42	Predictive approach for the design of improved HDT catalysts: Î³-Alumina supported (Ni, Co) promoted Mo1â^'xWxS2 active phases. Applied Catalysis A: General, 2007, 322, 92-97.	4.3	79
43	Aging of Co(Ni)MoP/Al2O3 catalysts in working state. Catalysis Today, 2008, 130, 97-108.	4.4	78
44	Anionic or Cationic S-Doping in Bulk Anatase TiO₂: Insights on Optical Absorption from First Principles Calculations. Journal of Physical Chemistry C, 2013, 117, 8892-8902.	3.1	78
45	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
46	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
47	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
48	Theoretical Unraveling of Selective 1-Butene Oligomerization Catalyzed by Ironâ^'Bis(arylimino)pyridine. Organometallics, 2009, 28, 5358-5367.	2.3	72
49	Effects of PH2O, PH2S, PH2 on the surface properties of anatase?TiO2 and ?-Al2O3: a DFT study. Journal of Catalysis, 2004, 226, 260-272.	6.2	69
50	Quantitative Two-Dimensional (2D) Morphologyâ€“Selectivity Relationship of CoMoS Nanolayers: A Combined High-Resolution High-Angle Annular Dark Field Scanning Transmission Electron Microscopy (HR HAADF-STEM) and Density Functional Theory (DFT) Study. ACS Catalysis, 2016, 6, 1081-1092.	11.2	67
51	A DFT study of the origin of the HDS/HydO selectivity on Co(Ni)MoS active phases. Journal of Catalysis, 2008, 260, 276-287.	6.2	66
52	DFT makes the morphologies of anatase-TiO2 nanoparticles visible to IR spectroscopy. Journal of Catalysis, 2005, 236, 245-250.	6.2	63
53	New insights into parameters controlling the selectivity in hydrocracking reactions. Journal of Catalysis, 2003, 217, 376-387.	6.2	62
54	Atomic Scale Insights on Chlorinated Î³-Alumina Surfaces. Journal of the American Chemical Society, 2008, 130, 11030-11039.	13.7	61

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55	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
56	Acidity of Amorphous Silicaâ€“Alumina: From Coordination Promotion of Lewis Sites to Proton Transfer. ChemPhysChem, 2010, 11, 105-108.	2.1	56
57	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
58	Cobalt Catalyzed Fischerâ€“Tropsch Synthesis: Perspectives Opened by First Principles Calculations. Catalysis Letters, 2013, 143, 1-17.	2.6	53
59	Tuning the Magnetic Properties of MoS₂ Single Nanolayers by 3d Metals Edge Doping. Journal of Physical Chemistry C, 2016, 120, 10691-10697.	3.1	52
60	Competitive adsorption of nitrogen and sulphur compounds on a multisite model of NiMoS catalyst: A theoretical study. Journal of Catalysis, 2016, 333, 78-93.	6.2	52
61	Periodic trends in the selective hydrogenation of styrene over silica supported metal catalysts. Journal of Catalysis, 2013, 307, 352-361.	6.2	51
62	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
63	Dehydrogenation mechanisms of methyl-cyclohexane on Î³-Al2O3 supported Pt13: Impact of cluster ductility. Journal of Catalysis, 2019, 370, 118-129.	6.2	47
64	Potassium Silanide (KSiH₃): A Reversible Hydrogen Storage Material. Chemistry - A European Journal, 2011, 17, 12302-12309.	3.3	46
65	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
66	THERMIDOR: A new model for combined simulation of operations and optimization of catalysts in residues hydroprocessing units. Catalysis Today, 2005, 109, 135-153.	4.4	44
67	On the understanding of the optoelectronic properties of S-doped MoO₃ and O-doped MoS₂ bulk systems: a DFT perspective. Journal of Materials Chemistry C, 2020, 8, 9064-9074.	5.5	44
68	A QSPR Investigation of Thermal Stability of [Al(CH3)O]n Oligomers in Methylaluminoxane Solution: The Identification of a Geometry-Based Descriptor. Organometallics, 2012, 31, 8312-8322.	2.3	43
69	Comment on â€œExamination of Spinel and Nonspinel Structural Models for Î³-Al2O3by DFT and Rietveld Refinement Simulationsâ€. Journal of Physical Chemistry B, 2006, 110, 20719-20720.	2.6	42
70	Transformation of a model FCC gasoline olefin over transition monometallic sulfide catalysts. Journal of Catalysis, 2007, 248, 111-119.	6.2	42
71	Microkinetic interpretation of HDS/HYDO selectivity of the transformation of a model FCC gasoline over transition metal sulfides. Catalysis Today, 2008, 130, 221-230.	4.4	40
72	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

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73	Highly Active Nonpromoted Hydrotreating Catalysts through the Controlled Growth of a Supported Hexagonal WS₂ Phase. ACS Catalysis, 2014, 4, 4320-4331.	11.2	39
74	Evidence for the Iron(III) Oxidation State in Bis(imino)pyridine Catalysts. A Density Functional Theory Study. Organometallics, 2008, 27, 3368-3377.	2.3	38
75	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
76	A rational interpretation of improved catalytic performances of additive-impregnated dried CoMo hydrotreating catalysts: a combined theoretical and experimental study. Catalysis Science and Technology, 2013, 3, 140-151.	4.1	37
77	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
78	Temperature-programed reduction of unpromoted MoS2-based hydrodesulfurization catalysts: Experiments and kinetic modeling from first principles. Journal of Catalysis, 2009, 267, 67-77.	6.2	35
79	CO adsorption on amorphous silicaâ€“alumina: electrostatic or BrÃ¸nsted acidity probe?. Chemical Communications, 2012, 48, 4076.	4.1	35
80	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
81	Effects of zeolite pore sizes on the mechanism and selectivity ofÂxyleneÂdisproportionationâ€”a DFT study. Journal of Catalysis, 2004, 222, 323-337.	6.2	34
82	A Rational Comparison of the Optimal Promoter Edge Decoration of HDT NiMoS vs CoMoS Catalysts. Oil and Gas Science and Technology, 2009, 64, 719-730.	1.4	34
83	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
84	An Atomistic Description of the Î³-Alumina/Water Interface Revealed by Ab Initio Molecular Dynamics. Journal of Physical Chemistry C, 2017, 121, 10351-10363.	3.1	33
85	Effect of confinement on the selectivity of hydrocracking. Journal of Catalysis, 2004, 221, 500-509.	6.2	32
86	Abâ€…Initio Simulation of the Acid Sites at the External Surface of Zeolite Beta. ChemCatChem, 2017, 9, 2176-2185.	3.7	32
87	Structural, energetic, and electronic trends in low-dimensional late-transition-metal systems. Physical Review B, 2009, 79, .	3.2	31
88	A DFT Study of CoMoS and NiMoS Catalysts: from Nano-Crystallite Morphology to Selective Hydrodesulfurization. Oil and Gas Science and Technology, 2009, 64, 707-718.	1.4	30
89	Stability of Carbon on Cobalt Surfaces in Fischerâ€“Tropsch Reaction Conditions: A DFT Study. Journal of Physical Chemistry C, 2014, 118, 22479-22490.	3.1	30
90	Tuning the Metalâ€“Support Interaction by Structural Recognition of Cobaltâ€Based Catalyst Precursors. Angewandte Chemie - International Edition, 2015, 54, 6824-6827.	13.8	30

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91	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
92	Enthalpyâ€“Entropy Compensation Effect in Hydrogen Storage Materials: Striking Example of Alkali Silanides MSiH3(M = K, Rb, Cs). Journal of Physical Chemistry C, 2014, 118, 3409-3419.	3.1	29
93	2D MoO_{3â€“x}S_x/MoS₂van der Waals Assembly: A Tunable Heterojunction with Attractive Properties for Photocatalysis. ACS Applied Materials & Interfaces, 2021, 13, 36465-36474.	8.0	29
94	Understanding the role of aluminum-based activators in single site iron catalysts for ethylene oligomerization. Journal of Catalysis, 2014, 317, 153-157.	6.2	28
95	Deep HDS of FCC gasoline over alumina supported CoMoS catalyst: Inhibiting effects of carbon monoxide and water. Applied Catalysis B: Environmental, 2016, 183, 317-327.	20.2	28
96	Improved promoter effect in NiWS catalysts through a molecular approach and an optimized Ni edge decoration. Journal of Catalysis, 2016, 340, 60-65.	6.2	27
97	Quantum chemical and vibrational investigation of sodium exchanged Î³-alumina surfaces. Physical Chemistry Chemical Physics, 2007, 9, 2577-2582.	2.8	26
98	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
99	A DFT Chemical Descriptor to Predict the Selectivity in Î±-Olefins in the Catalytic Metallacyclic Oligomerization Reaction of Ethylene According to the (Hemi)labile Ligand Coordinating to Titanium. Organometallics, 2008, 27, 4864-4872.	2.3	24
100	Dual Effect of H2S on Volcano Curves in Hydrotreating Sulfide Catalysis. Oil and Gas Science and Technology, 2006, 61, 515-525.	1.4	22
101	First principles surface thermodynamics of industrial supported catalysts in working conditions. Journal of Physics Condensed Matter, 2008, 20, 064235.	1.8	21
102	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
103	Temperature-programmed reduction of unpromoted MoS2-based hydrodesulfurization catalysts: First-principles kinetic Monte Carlo simulations and comparison with experiments. Journal of Catalysis, 2010, 275, 117-128.	6.2	20
104	Active sites speciation of supported CoMoS phase probed by NO molecule: A combined IR and DFT study. Journal of Catalysis, 2018, 361, 62-72.	6.2	20
105	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
106	Hydrogenation properties of KSi and NaSi Zintl phases. Physical Chemistry Chemical Physics, 2012, 14, 13319.	2.8	19
107	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
108	Iron bis(arylimino)pyridine precursors activated to catalyze ethylene oligomerization as studied by DFT and QSAR approaches. Computational and Theoretical Chemistry, 2009, 903, 100-107.	1.5	17

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109	Magnifying the Morphology Change Induced by a Nickel Promoter in Tungsten(IV) Sulfide Industrial Hydrocracking Catalyst: A HAADFâ€STEM and DFT Study. ChemCatChem, 2014, 6, 1594-1598.	3.7	17
110	Thermokinetic and Spectroscopic Mapping of Carbon Monoxide Adsorption on Highly Dispersed Pt/Î³-Al₂O₃. ACS Catalysis, 2021, 11, 13280-13293.	11.2	17
111	Thermodynamic Properties of Trialkali (Li, Na, K) Hexa-alanates: A Combined DFT and Experimental Study. Journal of Physical Chemistry C, 2008, 112, 18598-18607.	3.1	15
112	Compensation effect and volcano curve in toluene hydrogenation catalyzed by transition metal sulfides. Dalton Transactions, 2010, 39, 8420.	3.3	15
113	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
114	Adsorption of NO on Pd-Exchanged Mordenite: Ab Initio DFT Modeling. Journal of Physical Chemistry C, 2008, 112, 12349-12362.	3.1	13
115	Prediction of optimal catalysts for a given chemical reaction. Catalysis Science and Technology, 2020, 10, 2069-2081.	4.1	13
116	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
117	Computational chemistry approaches for the preparation of supported catalysts: Progress and challenges. Journal of Catalysis, 2020, 391, 539-547.	6.2	12
118	Topological Analysis of the Interactions between Organic Molecules and Co(Ni)MoS Catalytic Active Phases. Journal of Chemical Theory and Computation, 2009, 5, 580-593.	5.3	11
119	Impact of CO on the transformation of a model FCC gasoline over CoMoS/Al2O3 catalysts: A combined kinetic and DFT approach. Applied Catalysis B: Environmental, 2010, 97, 323-332.	20.2	11
120	In Silico Prediction of Catalytic Oligomerization Degrees. Organometallics, 2011, 30, 3911-3914.	2.3	11
121	Surface speciation of Co based Fischer-Tropsch catalyst under reaction conditions: Deactivation by coke or by oxidation?. Applied Catalysis A: General, 2020, 590, 117332.	4.3	9
122	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
123	Size-Dependent Structural, Energetic, and Spectroscopic Properties of MoS₃ Polymorphs. Crystal Growth and Design, 2020, 20, 7750-7760.	3.0	9
124	Evidence for H₂-Induced Ductility in a Pt/Al₂O₃ Catalyst. ACS Catalysis, 2022, 12, 5979-5989.	11.2	9
125	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
126	Theoretical Insights into the Interaction of Oxygenated Organic Molecules and Cobalt(II) Precursor with Î³-Al₂O₃Surfaces. Journal of Physical Chemistry C, 2018, 122, 19560-19574.	3.1	8

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127	Combined Experimental and Theoretical Molecular Approach of the Catalytically Active Hydrotreating MoS₂ Phases Promoted by 3d Transition Metals. Journal of Physical Chemistry C, 2019, 123, 24659-24669.	3.1	8
128	Competitive Deposition of C and O Species on Cobalt Surface in Fischerâ€“Tropsch Synthesis Conditions: A Plausible Origin of Deactivation. Journal of Physical Chemistry C, 2015, 119, 23515-23526.	3.1	7
129	Electronic structures of the MoS₂/TiO₂(anatase) heterojunction: influence of physical and chemical modifications at the 2D- or 1D-interfaces. Physical Chemistry Chemical Physics, 2022, 24, 2646-2655.	2.8	6
130	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
131	Genesis of MoS2 from model-Mo-oxide precursors supported on Î³-alumina. Journal of Catalysis, 2022, 408, 303-315.	6.2	4
132	Structural Characterization of Phosphate Species Adsorbed on Î³-Alumina by Combining DNP Surface Enhanced NMR Spectroscopy and DFT Calculations. ACS Catalysis, 2021, 11, 11278-11292.	11.2	3
133	Hydrogenolysis and Î²â€“elimination mechanisms for C S bond scission of dibenzothiophene on CoMoS edge sites. Journal of Catalysis, 2021, 403, 32-42.	6.2	1