

Pascal Raybaud

List of Publications by Year in descending order

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papers

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28190

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140
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140
docs citations

140
times ranked

8526
citing authors

#	ARTICLE	IF	CITATIONS
1	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.	5.5	21
2	Electronic structures of the MoS ₂ /TiO ₂ (anatase) heterojunction: influence of physical and chemical modifications at the 2D- or 1D-interfaces. Physical Chemistry Chemical Physics, 2022, 24, 2646-2655.	1.3	6
3	Genesis of MoS ₂ from model-Mo-oxide precursors supported on γ -alumina. Journal of Catalysis, 2022, 408, 303-315.	3.1	4
4	Evidence for H ₂ -Induced Ductility in a Pt/Al ₂ O ₃ Catalyst. ACS Catalysis, 2022, 12, 5979-5989.	5.5	9
5	Evaluating acid and metallic site proximity in Pt/ γ -Al ₂ O ₃ -Cl bifunctional catalysts through an atomic scale geometrical model. Nanoscale, 2022, 14, 8753-8765.	2.8	6
6	Hydrogenolysis and β -elimination mechanisms for C-S bond scission of dibenzothiophene on CoMoS edge sites. Journal of Catalysis, 2021, 403, 32-42.	3.1	1
7	2D MoO ₃ -xS _x /MoS ₂ van der Waals Assembly: A Tunable Heterojunction with Attractive Properties for Photocatalysis. ACS Applied Materials & Interfaces, 2021, 13, 36465-36474.	4.0	29
8	Structural Characterization of Phosphate Species Adsorbed on γ -Alumina by Combining DNP Surface Enhanced NMR Spectroscopy and DFT Calculations. ACS Catalysis, 2021, 11, 11278-11292.	5.5	3
9	Thermokinetic and Spectroscopic Mapping of Carbon Monoxide Adsorption on Highly Dispersed Pt/ γ -Al ₂ O ₃ . ACS Catalysis, 2021, 11, 13280-13293.	5.5	17
10	Surface speciation of Co based Fischer-Tropsch catalyst under reaction conditions: Deactivation by coke or by oxidation?. Applied Catalysis A: General, 2020, 590, 117332.	2.2	9
11	Computational chemistry approaches for the preparation of supported catalysts: Progress and challenges. Journal of Catalysis, 2020, 391, 539-547.	3.1	12
12	Dynamic Features of Transition States for β -Scission Reactions of Alkenes over Acid Zeolites Revealed by AIMD Simulations. Angewandte Chemie, 2020, 132, 19100-19104.	1.6	9
13	Size-Dependent Structural, Energetic, and Spectroscopic Properties of MoS ₃ Polymorphs. Crystal Growth and Design, 2020, 20, 7750-7760.	1.4	9
14	On the understanding of the optoelectronic properties of S-doped MoO ₃ and O-doped MoS ₂ bulk systems: a DFT perspective. Journal of Materials Chemistry C, 2020, 8, 9064-9074.	2.7	44
15	Dynamic Features of Transition States for β -Scission Reactions of Alkenes over Acid Zeolites Revealed by AIMD Simulations. Angewandte Chemie - International Edition, 2020, 59, 18938-18942.	7.2	20
16	Atomic Scale Insight into the Formation, Size, and Location of Platinum Nanoparticles Supported on γ -Alumina. ACS Catalysis, 2020, 10, 4193-4204.	5.5	30
17	Prediction of optimal catalysts for a given chemical reaction. Catalysis Science and Technology, 2020, 10, 2069-2081.	2.1	13
18	Interplay of the adsorption of light and heavy paraffins in hydroisomerization over H-beta zeolite. Catalysis Science and Technology, 2019, 9, 5368-5382.	2.1	12

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19	Combined Experimental and Theoretical Molecular Approach of the Catalytically Active Hydrotreating MoS ₂ Phases Promoted by 3d Transition Metals. Journal of Physical Chemistry C, 2019, 123, 24659-24669.	1.5	8
20	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.	5.5	35
21	Beyond γ -Al ₂ O ₃ crystallite surfaces: The hidden features of edges revealed by solid-state ¹ H NMR and DFT calculations. Journal of Catalysis, 2019, 378, 140-143.	3.1	36
22	Atomistic Models for Highly Dispersed PtSn/ γ -Al ₂ O ₃ Catalysts: Ductility and Dilution Affect the Affinity for Hydrogen. ChemCatChem, 2019, 11, 3941-3951.	1.8	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.	3.1	38
24	Dehydrogenation mechanisms of methyl-cyclohexane on γ -Al ₂ O ₃ supported Pt ₁₃ : Impact of cluster ductility. Journal of Catalysis, 2019, 370, 118-129.	3.1	47
25	Active sites speciation of supported CoMoS phase probed by NO molecule: A combined IR and DFT study. Journal of Catalysis, 2018, 361, 62-72.	3.1	20
26	Theoretical Insights into the Interaction of Oxygenated Organic Molecules and Cobalt(II) Precursor with γ -Al ₂ O ₃ Surfaces. Journal of Physical Chemistry C, 2018, 122, 19560-19574.	1.5	8
27	Ab Initio Simulation of the Acid Sites at the External Surface of Zeolite Beta. ChemCatChem, 2017, 9, 2176-2185.	1.8	32
28	An Atomistic Description of the γ -Alumina/Water Interface Revealed by Ab Initio Molecular Dynamics. Journal of Physical Chemistry C, 2017, 121, 10351-10363.	1.5	33
29	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
30	Dealumination mechanisms of zeolites and extra-framework aluminum confinement. Journal of Catalysis, 2016, 339, 242-255.	3.1	149
31	Tuning the Magnetic Properties of MoS ₂ Single Nanolayers by 3d Metals Edge Doping. Journal of Physical Chemistry C, 2016, 120, 10691-10697.	1.5	52
32	Improved promoter effect in NiWS catalysts through a molecular approach and an optimized Ni edge decoration. Journal of Catalysis, 2016, 340, 60-65.	3.1	27
33	Quantitative Two-Dimensional (2D) Morphology-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.	5.5	67
34	Competitive adsorption of nitrogen and sulphur compounds on a multisite model of NiMoS catalyst: A theoretical study. Journal of Catalysis, 2016, 333, 78-93.	3.1	52
35	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.	10.8	28
36	Tuning the Metal-Support Interaction by Structural Recognition of Cobalt-Based Catalyst Precursors. Angewandte Chemie - International Edition, 2015, 54, 6824-6827.	7.2	30

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37	Revisiting carbenium chemistry on amorphous silica-alumina: Unraveling their milder acidity as compared to zeolites. <i>Journal of Catalysis</i> , 2015, 325, 35-47.	3.1	45
38	Competitive Deposition of C and O Species on Cobalt Surface in Fischer-Tropsch Synthesis Conditions: A Plausible Origin of Deactivation. <i>Journal of Physical Chemistry C</i> , 2015, 119, 23515-23526.	1.5	7
39	Atomic Description of the Interface between Silica and Alumina in Aluminosilicates through Dynamic Nuclear Polarization Surface-Enhanced NMR Spectroscopy and First-Principles Calculations. <i>Journal of the American Chemical Society</i> , 2015, 137, 10710-10719.	6.6	129
40	Regioselectivity of Al-O Bond Hydrolysis during Zeolites Dealumination Unified by Brønsted-Evans-Polanyi Relationship. <i>ACS Catalysis</i> , 2015, 5, 11-15.	5.5	73
41	Highly Active Nonpromoted Hydrotreating Catalysts through the Controlled Growth of a Supported Hexagonal WS ₂ Phase. <i>ACS Catalysis</i> , 2014, 4, 4320-4331.	5.5	39
42	Challenges on molecular aspects of dealumination and desilication of zeolites. <i>Microporous and Mesoporous Materials</i> , 2014, 191, 82-96.	2.2	240
43	Magnifying the Morphology Change Induced by a Nickel Promoter in Tungsten(IV) Sulfide Industrial Hydrocracking Catalyst: A HAADF-STEM and DFT Study. <i>ChemCatChem</i> , 2014, 6, 1594-1598.	1.8	17
44	Tuning the properties of visible-light-responsive tantalum (oxy)nitride photocatalysts by non-stoichiometric compositions: a first-principles viewpoint. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 20548-20560.	1.3	86
45	Stability of Carbon on Cobalt Surfaces in Fischer-Tropsch Reaction Conditions: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22479-22490.	1.5	30
46	Enthalpy-Entropy Compensation Effect in Hydrogen Storage Materials: Striking Example of Alkali Silanides MSiH ₃ (M = K, Rb, Cs). <i>Journal of Physical Chemistry C</i> , 2014, 118, 3409-3419.	1.5	29
47	Understanding the role of aluminum-based activators in single site iron catalysts for ethylene oligomerization. <i>Journal of Catalysis</i> , 2014, 317, 153-157.	3.1	28
48	Density functional theory simulations of complex catalytic materials in reactive environments: beyond the ideal surface at low coverage. <i>Catalysis Science and Technology</i> , 2014, 4, 2797-2813.	2.1	57
49	Monitoring Morphology and Hydrogen Coverage of Nanometric Pt/Al ₂ O ₃ Particles by In-Situ HERFD-XANES and Quantum Simulations. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 12426-12429.	7.2	47
50	From γ-alumina to supported platinum nanoclusters in reforming conditions: 10 years of DFT modeling and beyond. <i>Journal of Catalysis</i> , 2013, 308, 328-340.	3.1	73
51	Periodic trends in the selective hydrogenation of styrene over silica supported metal catalysts. <i>Journal of Catalysis</i> , 2013, 307, 352-361.	3.1	51
52	A rational interpretation of improved catalytic performances of additive-impregnated dried CoMo hydrotreating catalysts: a combined theoretical and experimental study. <i>Catalysis Science and Technology</i> , 2013, 3, 140-151.	2.1	37
53	Cobalt Catalyzed Fischer-Tropsch Synthesis: Perspectives Opened by First Principles Calculations. <i>Catalysis Letters</i> , 2013, 143, 1-17.	1.4	53
54	Anionic or Cationic S-Doping in Bulk Anatase TiO ₂ : Insights on Optical Absorption from First Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2013, 117, 8892-8902.	1.5	78

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55	Comment on “Electronic properties and charge transfer phenomena in Pt nanoparticles on γ -Al ₂ O ₃ : size, shape, support, and adsorbate effects” by F. Behafarid et al., Phys. Chem. Chem. Phys., 2012, 14, 11766–11779. Physical Chemistry Chemical Physics, 2012, 14, 16773.	1.3	8
56	Hydrogenation properties of KSi and NaSi Zintl phases. Physical Chemistry Chemical Physics, 2012, 14, 13319.	1.3	19
57	A QSPR Investigation of Thermal Stability of [Al(CH ₃ O) _n] Oligomers in Methylaluminoxane Solution: The Identification of a Geometry-Based Descriptor. Organometallics, 2012, 31, 8312-8322.	1.1	43
58	Effect of Indium Doping of γ -Alumina on the Stabilization of PtSn Alloyed Clusters Prepared by Surface Organostannic Chemistry. Journal of Physical Chemistry C, 2012, 116, 10073-10083.	1.5	25
59	Platinum Nanoclusters Stabilized on γ -Alumina by Chlorine Used As a Capping Surface Ligand: A Density Functional Theory Study. ACS Catalysis, 2012, 2, 1346-1357.	5.5	77
60	CO adsorption on amorphous silica–alumina: electrostatic or Brønsted acidity probe?. Chemical Communications, 2012, 48, 4076.	2.2	35
61	Deoxygenation mechanisms on Ni-promoted MoS ₂ bulk catalysts: A combined experimental and theoretical study. Journal of Catalysis, 2012, 286, 153-164.	3.1	107
62	Thermodynamic Stability of Buta-1,3-diene and But-1-ene on Pd(111) and (100) Surfaces under H ₂ Pressure: A DFT Study. Journal of Physical Chemistry C, 2011, 115, 12135-12149.	1.5	40
63	Origin of the Enhanced Visible-Light Absorption in N-Doped Bulk Anatase TiO ₂ from First-Principles Calculations. Journal of Physical Chemistry C, 2011, 115, 19394-19404.	1.5	91
64	<i>In Silico</i> Prediction of Catalytic Oligomerization Degrees. Organometallics, 2011, 30, 3911-3914.	1.1	11
65	Hydrodeoxygenation pathways catalyzed by MoS ₂ and NiMoS active phases: A DFT study. Journal of Catalysis, 2011, 279, 276-286.	3.1	118
66	Free-energy profiles along reduction pathways of MoS ₂ M-edge and S-edge by dihydrogen: A first-principles study. Journal of Catalysis, 2011, 280, 178-195.	3.1	117
67	Brønsted acidity of amorphous silica–alumina: The molecular rules of proton transfer. Journal of Catalysis, 2011, 284, 215-229.	3.1	96
68	H ₂ -Induced Reconstruction of Supported Pt Clusters: Metal–Support Interaction versus Surface Hydride. ChemCatChem, 2011, 3, 200-207.	1.8	152
69	Potassium Silanide (KSiH ₃): A Reversible Hydrogen Storage Material. Chemistry - A European Journal, 2011, 17, 12302-12309.	1.7	46
70	Modulation of catalyst particle structure upon support hydroxylation: Ab initio insights into Pd ₁₃ and Pt ₁₃ / γ -Al ₂ O ₃ . Journal of Catalysis, 2010, 274, 99-110.	3.1	137
71	Temperature-programmed reduction of unpromoted MoS ₂ -based hydrodesulfurization catalysts: First-principles kinetic Monte Carlo simulations and comparison with experiments. Journal of Catalysis, 2010, 275, 117-128.	3.1	20
72	Acidity of Amorphous Silica–Alumina: From Coordination Promotion of Lewis Sites to Proton Transfer. ChemPhysChem, 2010, 11, 105-108.	1.0	56

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73	Impact of CO on the transformation of a model FCC gasoline over CoMoS/Al ₂ O ₃ catalysts: A combined kinetic and DFT approach. Applied Catalysis B: Environmental, 2010, 97, 323-332.	10.8	11
74	Compensation effect and volcano curve in toluene hydrogenation catalyzed by transition metal sulfides. Dalton Transactions, 2010, 39, 8420.	1.6	15
75	The role of the extra-framework cations in the adsorption of CO ₂ on faujasite Y. Physical Chemistry Chemical Physics, 2010, 12, 13534.	1.3	117
76	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
77	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
78	Structural, energetic, and electronic trends in low-dimensional late-transition-metal systems. Physical Review B, 2009, 79, .	1.1	31
79	Temperature-programed reduction of unpromoted MoS ₂ -based hydrodesulfurization catalysts: Experiments and kinetic modeling from first principles. Journal of Catalysis, 2009, 267, 67-77.	3.1	35
80	Pseudo- π -Bridging Silanols as Versatile Brønsted Acid Sites of Amorphous Aluminosilicate Surfaces. Angewandte Chemie - International Edition, 2009, 48, 2891-2893.	7.2	109
81	Insights into the Geometry, Stability and Vibrational Properties of OH Groups on γ -Al ₂ O ₃ , TiO ₂ -Anatase and MgO from DFT Calculations. Topics in Catalysis, 2009, 52, 1005-1016.	1.3	34
82	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
83	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.	2.3	11
84	Theoretical Unraveling of Selective 1-Butene Oligomerization Catalyzed by Iron-Bis(arylimino)pyridine. Organometallics, 2009, 28, 5358-5367.	1.1	72
85	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.	1.3	53
86	Optimal promoter edge decoration of CoMoS catalysts: A combined theoretical and experimental study. Catalysis Today, 2008, 130, 149-159.	2.2	184
87	Microkinetic interpretation of HDS/HYDO selectivity of the transformation of a model FCC gasoline over transition metal sulfides. Catalysis Today, 2008, 130, 221-230.	2.2	40
88	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.	2.2	147
89	Aging of Co(Ni)MoP/Al ₂ O ₃ catalysts in working state. Catalysis Today, 2008, 130, 97-108.	2.2	78
90	A DFT study of the origin of the HDS/HydO selectivity on Co(Ni)MoS active phases. Journal of Catalysis, 2008, 260, 276-287.	3.1	66

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91	A DFT Chemical Descriptor to Predict the Selectivity in $\hat{\text{I}}^{\pm}$ -Olefins in the Catalytic Metallacyclic Oligomerization Reaction of Ethylene According to the (Hemi)labile Ligand Coordinating to Titanium. <i>Organometallics</i> , 2008, 27, 4864-4872.	1.1	24
92	Atomic Scale Insights on Chlorinated $\hat{\text{I}}^3$ -Alumina Surfaces. <i>Journal of the American Chemical Society</i> , 2008, 130, 11030-11039.	6.6	61
93	Evidence for the Iron(III) Oxidation State in Bis(imino)pyridine Catalysts. A Density Functional Theory Study. <i>Organometallics</i> , 2008, 27, 3368-3377.	1.1	38
94	First principles surface thermodynamics of industrial supported catalysts in working conditions. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 064235.	0.7	21
95	Thermodynamic Properties of Trialkali (Li, Na, K) Hexa-alanates: A Combined DFT and Experimental Study. <i>Journal of Physical Chemistry C</i> , 2008, 112, 18598-18607.	1.5	15
96	Adsorption of NO on Pd-Exchanged Mordenite: Ab Initio DFT Modeling. <i>Journal of Physical Chemistry C</i> , 2008, 112, 12349-12362.	1.5	13
97	Nucleation of Pd_n ($n=1\text{--}5$) clusters and wetting of Pd particles on $\hat{\text{I}}^3\text{-Al}_2\text{O}_3$ surfaces: A density functional theory study. <i>Physical Review B</i> , 2007, 75, .	1.1	84
98	Quantum chemical and vibrational investigation of sodium exchanged $\hat{\text{I}}^3$ -alumina surfaces. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 2577-2582.	1.3	26
99	Predictive approach for the design of improved HDT catalysts: $\hat{\text{I}}^3$ -Alumina supported (Ni, Co) promoted $\text{Mo}_{1-x}\text{W}_x\text{S}_2$ active phases. <i>Applied Catalysis A: General</i> , 2007, 322, 92-97.	2.2	79
100	Understanding and predicting improved sulfide catalysts: Insights from first principles modeling. <i>Applied Catalysis A: General</i> , 2007, 322, 76-91.	2.2	136
101	Edge wetting effects of $\hat{\text{I}}^3\text{-Al}_2\text{O}_3$ and anatase- TiO_2 supports by MoS_2 and CoMoS active phases: A DFT study. <i>Journal of Catalysis</i> , 2007, 246, 325-343.	3.1	87
102	Interplay between molecular adsorption and metal-support interaction for small supported metal clusters: CO and C_2H_4 adsorption on $\text{Pd}_4/\hat{\text{I}}^3\text{Pd}_4/\hat{\text{I}}^3\text{-Al}_2\text{O}_3$. <i>Journal of Catalysis</i> , 2007, 247, 339-355.	3.1	80
103	Transformation of a model FCC gasoline olefin over transition monometallic sulfide catalysts. <i>Journal of Catalysis</i> , 2007, 248, 111-119.	3.1	42
104	Influence of the Hydroxylation of $\hat{\text{I}}^3\text{-Al}_2\text{O}_3$ Surfaces on the Stability and Diffusion of Single Pd Atoms: A DFT Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 1759-1767.	1.2	103
105	Comment on "Examination of Spinel and Nonspinel Structural Models for $\hat{\text{I}}^3\text{-Al}_2\text{O}_3$ by DFT and Rietveld Refinement Simulations". <i>Journal of Physical Chemistry B</i> , 2006, 110, 20719-20720.	1.2	42
106	Dual Effect of H_2S on Volcano Curves in Hydrotreating Sulfide Catalysis. <i>Oil and Gas Science and Technology</i> , 2006, 61, 515-525.	1.4	22
107	A density functional theory comparison of anatase (TiO_2)- and $\hat{\text{I}}^3\text{-Al}_2\text{O}_3$ -supported MoS_2 catalysts. <i>Journal of Catalysis</i> , 2005, 232, 161-178.	3.1	105
108	DFT makes the morphologies of anatase- TiO_2 nanoparticles visible to IR spectroscopy. <i>Journal of Catalysis</i> , 2005, 236, 245-250.	3.1	63

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109	THERMIDOR: A new model for combined simulation of operations and optimization of catalysts in residues hydroprocessing units. <i>Catalysis Today</i> , 2005, 109, 135-153.	2.2	44
110	Effect of confinement on the selectivity of hydrocracking. <i>Journal of Catalysis</i> , 2004, 221, 500-509.	3.1	32
111	Use of DFT to achieve a rational understanding of acid/basic properties of γ -alumina surfaces. <i>Journal of Catalysis</i> , 2004, 226, 54-68.	3.1	880
112	Effects of PH ₂ O, PH ₂ S, PH ₂ on the surface properties of anatase-TiO ₂ and γ -Al ₂ O ₃ : a DFT study. <i>Journal of Catalysis</i> , 2004, 226, 260-272.	3.1	69
113	Effects of morphology on surface hydroxyl concentration: a DFT comparison of anatase-TiO ₂ and γ -alumina catalytic supports. <i>Journal of Catalysis</i> , 2004, 222, 152-166.	3.1	300
114	Effects of zeolite pore sizes on the mechanism and selectivity of α -xylene disproportionation: a DFT study. <i>Journal of Catalysis</i> , 2004, 222, 323-337.	3.1	34
115	Kinetic interpretation of catalytic activity patterns based on theoretical chemical descriptors. <i>Journal of Catalysis</i> , 2003, 216, 63-72.	3.1	165
116	New insights into parameters controlling the selectivity in hydrocracking reactions. <i>Journal of Catalysis</i> , 2003, 217, 376-387.	3.1	62
117	Adsorption of Unsaturated Hydrocarbons on Pd(111) and Pt(111): A DFT Study. <i>Journal of Physical Chemistry B</i> , 2003, 107, 12287-12295.	1.2	148
118	Hemilabile Ligand Induced Selectivity: a DFT Study on Ethylene Trimerization Catalyzed by Titanium Complexes. <i>Organometallics</i> , 2003, 22, 3404-3413.	1.1	109
119	Structure and Stability of Aluminum Hydroxides: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2002, 106, 5155-5162.	1.2	241
120	Periodic trends in hydrodesulfurization: in support of the Sabatier principle. <i>Applied Catalysis A: General</i> , 2002, 227, 83-96.	2.2	189
121	Shape and Edge Sites Modifications of MoS ₂ Catalytic Nanoparticles Induced by Working Conditions: A Theoretical Study. <i>Journal of Catalysis</i> , 2002, 207, 76-87.	3.1	337
122	Promoter Sensitive Shapes of Co(Ni)MoS Nanocatalysts in Sulfo-Reductive Conditions. <i>Journal of Catalysis</i> , 2002, 212, 33-38.	3.1	173
123	Hydroxyl Groups on γ -Alumina Surfaces: A DFT Study. <i>Journal of Catalysis</i> , 2002, 211, 1-5.	3.1	364
124	Theoretical Study of the Dehydration Process of Boehmite to γ -Alumina. <i>Journal of Physical Chemistry B</i> , 2001, 105, 5121-5130.	1.2	435
125	The Origin of the C ₇ -Hydroconversion Selectivities on Y, β , ZSM-22, ZSM-23, and EU-1 Zeolites. <i>Journal of Catalysis</i> , 2001, 197, 98-112.	3.1	104
126	Morphology and Surface Properties of Boehmite (γ -AlOOH): A Density Functional Theory Study. <i>Journal of Catalysis</i> , 2001, 201, 236-246.	3.1	218

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127	Ab Initio Study of the H ₂ –H ₂ S/MoS ₂ Gas–Solid Interface: The Nature of the Catalytically Active Sites. Journal of Catalysis, 2000, 189, 129-146.	3.1	350
128	Structure, Energetics, and Electronic Properties of the Surface of a Promoted MoS ₂ Catalyst: An ab Initio Local Density Functional Study. Journal of Catalysis, 2000, 190, 128-143.	3.1	321
129	Transition metals to sulfur binding energies relationship to catalytic activities in HDS: back to Sabatier with first principle calculations ¹ This work has been undertaken within the "GdR Dynamique Moléculaire Quantique Appliquée à la Catalyse", a joint project of Centre National de la Recherche Scientifique, Technische Universität Wien, and Institut Français du Pétrole. ¹ Catalysis Today, 1999, 50, 629-636.	2.2	152
130	Structural and electronic properties of the MoS ₂ (101̄,0) edge-surface. Surface Science, 1998, 407, 237-250.	0.8	108
131	Adsorption of Thiophene on the Catalytically Active Surface of MoS ₂ : An ab Initio Local-Density-Functional Study. Physical Review Letters, 1998, 80, 1481-1484.	2.9	128
132	Ab initio density functional studies of transition-metal sulphides: II. Electronic structure. Journal of Physics Condensed Matter, 1997, 9, 11107-11140.	0.7	109
133	Ab initio density functional studies of transition-metal sulphides: I. Crystal structure and cohesive properties. Journal of Physics Condensed Matter, 1997, 9, 11085-11106.	0.7	118