Pascal Raybaud

List of Publications by Year in Descending Order

135 papers	8,846 citations	52 h-index	91 g-index
140 ext. papers	9,613 ext. citations	6.5 avg, IF	6.16 L-index

#	Paper	IF	Citations
135	Electronic structures of the MoS/TiO (anatase) heterojunction: influence of physical and chemical modifications at the 2D- or 1D-interfaces.. *Physical Chemistry Chemical Physics*, **2022**, 24, 2646-2655	3.6	2
134	Genesis of MoS2 from model-Mo-oxide precursors supported on alumina. *Journal of Catalysis*, **2022**, 408, 303-315	7.3	0
133	2D MoOS/MoS van der Waals Assembly: A Tunable Heterojunction with Attractive Properties for Photocatalysis. *ACS Applied Materials & Interfaces*, **2021**, 13, 36465-36474	9.5	6
132	Hydrogenolysis and elimination mechanisms for C S bond scission of dibenzothiophene on CoMoS edge sites. *Journal of Catalysis*, **2021**, 403, 32-32	7.3	
131	Structural Characterization of Phosphate Species Adsorbed on Alumina by Combining DNP Surface Enhanced NMR Spectroscopy and DFT Calculations. *ACS Catalysis*, **2021**, 11, 11278-11292	13.1	2
130	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	7.1	19
129	Dynamic Features of Transition States for Scission Reactions of Alkenes over Acid Zeolites Revealed by AIMD Simulations. *Angewandte Chemie - International Edition*, **2020**, 59, 18938-18942	16.4	10
128	Atomic Scale Insight into the Formation, Size, and Location of Platinum Nanoparticles Supported on Alumina. *ACS Catalysis*, **2020**, 10, 4193-4204	13.1	12
127	Prediction of optimal catalysts for a given chemical reaction. *Catalysis Science and Technology*, **2020** , 10, 2069-2081	5.5	6
126	Surface speciation of Co based Fischer-Tropsch catalyst under reaction conditions: Deactivation by coke or by oxidation?. *Applied Catalysis A: General*, **2020**, 590, 117332	5.1	5
125	Computational chemistry approaches for the preparation of supported catalysts: Progress and challenges. *Journal of Catalysis*, **2020**, 391, 539-547	7.3	5
124	Dynamic Features of Transition States for Scission Reactions of Alkenes over Acid Zeolites Revealed by AIMD Simulations. *Angewandte Chemie*, **2020**, 132, 19100-19104	3.6	2
123	Size-Dependent Structural, Energetic, and Spectroscopic Properties of MoS3 Polymorphs. *Crystal Growth and Design*, **2020**, 20, 7750-7760	3.5	2
122	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	3.8	6
121	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	13.1	18
120	Beyond Al2O3 crystallite surfaces: The hidden features of edges revealed by solid-state 1H NMR and DFT calculations. *Journal of Catalysis*, **2019**, 378, 140-143	7.3	20
119	Atomistic Models for Highly-Dispersed PtSn/Al2O3 Catalysts: Ductility and Dilution Affect the Affinity for Hydrogen. *ChemCatChem*, **2019**, 11, 3941-3951	5.2	9

118	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	7.3	20
117	Interplay of the adsorption of light and heavy paraffins in hydroisomerization over H-beta zeolite. *Catalysis Science and Technology*, **2019**, 9, 5368-5382	5.5	8
116	Dehydrogenation mechanisms of methyl-cyclohexane on Al2O3 supported Pt13: Impact of cluster ductility. *Journal of Catalysis*, **2019**, 370, 118-129	7.3	31
115	Active sites speciation of supported CoMoS phase probed by NO molecule: A combined IR and DFT study. *Journal of Catalysis*, **2018**, 361, 62-72	7.3	16
114	Theoretical Insights into the Interaction of Oxygenated Organic Molecules and Cobalt(II) Precursor with Al2O3 Surfaces. *Journal of Physical Chemistry C*, **2018**, 122, 19560-19574	3.8	7
113	Ab Initio Simulation of the Acid Sites at the External Surface of Zeolite Beta. *ChemCatChem*, **2017**, 9, 2176-2185	5.2	24
112	An Atomistic Description of the Alumina/Water Interface Revealed by Ab Initio Molecular Dynamics. *Journal of Physical Chemistry C*, **2017**, 121, 10351-10363	3.8	27
111	Improved promoter effect in NiWS catalysts through a molecular approach and an optimized Ni edge decoration. *Journal of Catalysis*, **2016**, 340, 60-65	7.3	22
110	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	13.1	56
109	Competitive adsorption of nitrogen and sulphur compounds on a multisite model of NiMoS catalyst: A theoretical study. *Journal of Catalysis*, **2016**, 333, 78-93	7.3	44
108	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	21.8	24
107	Catalytic Reforming: Methodology and Process Development for a Constant Optimisation and Performance Enhancement. *Oil and Gas Science and Technology*, **2016**, 71, 41	1.9	7
106	Dealumination mechanisms of zeolites and extra-framework aluminum confinement. *Journal of Catalysis*, **2016**, 339, 242-255	7.3	105
105	Tuning the Magnetic Properties of MoS2 Single Nanolayers by 3d Metals Edge Doping. *Journal of Physical Chemistry C*, **2016**, 120, 10691-10697	3.8	43
104	Revisiting carbenium chemistry on amorphous silica-alumina: Unraveling their milder acidity as compared to zeolites. *Journal of Catalysis*, **2015**, 325, 35-47	7.3	37
103	Competitive Deposition of C and O Species on Cobalt Surface in Fischer–Tropsch Synthesis Conditions: A Plausible Origin of Deactivation. *Journal of Physical Chemistry C*, **2015**, 119, 23515-23526	3.8	5
102	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, 10710-9	16.4	104
101	Regioselectivity of Al–O Bond Hydrolysis during Zeolites Dealumination Unified by Brønsted–Evans–Polanyi Relationship. *ACS Catalysis*, **2015**, 5, 11-15	13.1	56

100	Tuning the Metal–Support Interaction by Structural Recognition of Cobalt-Based Catalyst Precursors. *Angewandte Chemie*, **2015**, 127, 6928-6931	3.6	0
99	Tuning the metal-support interaction by structural recognition of cobalt-based catalyst precursors. *Angewandte Chemie - International Edition*, **2015**, 54, 6824-7	16.4	25
98	Challenges on molecular aspects of dealumination and desilication of zeolites. *Microporous and Mesoporous Materials*, **2014**, 191, 82-96	5.3	173
97	Magnifying the Morphology Change Induced by a Nickel Promoter in Tungsten(IV) Sulfide Industrial Hydrocracking Catalyst: A HAADF-STEM and DFT Study. *ChemCatChem*, **2014**, 6, 1594-1598	5.2	15
96	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, 20548-60	3.6	77
95	Stability of Carbon on Cobalt Surfaces in Fischer–Tropsch Reaction Conditions: A DFT Study. *Journal of Physical Chemistry C*, **2014**, 118, 22479-22490	3.8	28
94	Enthalpy–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	3.8	23
93	Understanding the role of aluminum-based activators in single site iron catalysts for ethylene oligomerization. *Journal of Catalysis*, **2014**, 317, 153-157	7.3	27
92	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	5.5	45
91	Monitoring Morphology and Hydrogen Coverage of Nanometric Pt/γ-Al2O3 Particles by In Situ HERFD-XANES and Quantum Simulations. *Angewandte Chemie*, **2014**, 126, 12634-12637	3.6	20
90	Monitoring morphology and hydrogen coverage of nanometric Pt/γ-Al2 O3 particles by in situ HERFD-XANES and quantum simulations. *Angewandte Chemie - International Edition*, **2014**, 53, 12426-9	16.4	20
89	Highly Active Nonpromoted Hydrotreating Catalysts through the Controlled Growth of a Supported Hexagonal WS2 Phase. *ACS Catalysis*, **2014**, 4, 4320-4331	13.1	35
88	From γ-alumina to supported platinum nanoclusters in reforming conditions: 10 years of DFT modeling and beyond. *Journal of Catalysis*, **2013**, 308, 328-340	7.3	52
87	Periodic trends in the selective hydrogenation of styrene over silica supported metal catalysts. *Journal of Catalysis*, **2013**, 307, 352-361	7.3	47
86	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	5.5	32
85	Cobalt Catalyzed Fischer–Tropsch Synthesis: Perspectives Opened by First Principles Calculations. *Catalysis Letters*, **2013**, 143, 1-17	2.8	52
84	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	3.8	70
83	Deoxygenation mechanisms on Ni-promoted MoS2 bulk catalysts: A combined experimental and theoretical study. *Journal of Catalysis*, **2012**, 286, 153-164	7.3	92

82	Comment on "Electronic properties and charge transfer phenomena in Pt nanoparticles on γ-Al2O3: 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, 16773-4	3.6	7
81	Hydrogenation properties of KSi and NaSi Zintl phases. *Physical Chemistry Chemical Physics*, **2012**, 14, 13319-24	3.6	18
80	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	3.8	40
79	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	3.8	20
78	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	13.1	62
77	CO adsorption on amorphous silica-alumina: electrostatic or Brønsted acidity probe?. *Chemical Communications*, **2012**, 48, 4076-8	5.8	32
76	In Silico Prediction of Catalytic Oligomerization Degrees. *Organometallics*, **2011**, 30, 3911-3914	3.8	9
75	Hydrodeoxygenation pathways catalyzed by MoS2 and NiMoS active phases: A DFT study. *Journal of Catalysis*, **2011**, 279, 276-286	7.3	94
74	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	7.3	105
73	Brønsted acidity of amorphous silica–alumina: The molecular rules of proton transfer. *Journal of Catalysis*, **2011**, 284, 215-229	7.3	87
72	H2-Induced Reconstruction of Supported Pt Clusters: Metal–Support Interaction versus Surface Hydride. *ChemCatChem*, **2011**, 3, 200-207	5.2	132
71	Potassium silanide (KSiH3): a reversible hydrogen storage material. *Chemistry - A European Journal*, **2011**, 17, 12302-9	4.8	38
70	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	3.8	37
69	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	3.8	86
68	Compensation effect and volcano curve in toluene hydrogenation catalyzed by transition metal sulfides. *Dalton Transactions*, **2010**, 39, 8420-2	4.3	14
67	The role of the extra-framework cations in the adsorption of CO(2) on faujasite Y. *Physical Chemistry Chemical Physics*, **2010**, 12, 13534-46	3.6	97
66	Modulation of catalyst particle structure upon support hydroxylation: Ab initio insights into Pd13 and Pt13/γ-Al2O3. *Journal of Catalysis*, **2010**, 274, 99-110	7.3	125
65	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	7.3	19

64	Acidity of amorphous silica-alumina: from coordination promotion of Lewis sites to proton transfer. *ChemPhysChem*, **2010**, 11, 105-8	3.2	49
63	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	21.8	11
62	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	1.9	32
61	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	1.9	30
60	Structural, energetic, and electronic trends in low-dimensional late-transition-metal systems. *Physical Review B*, **2009**, 79,	3.3	29
59	Temperature-programed reduction of unpromoted MoS2-based hydrodesulfurization catalysts: Experiments and kinetic modeling from first principles. *Journal of Catalysis*, **2009**, 267, 67-77	7.3	32
58	Pseudo-Bridging Silanols as Versatile Brønsted Acid Sites of Amorphous Aluminosilicate Surfaces. *Angewandte Chemie*, **2009**, 121, 2935-2937	3.6	18
57	Pseudo-bridging silanols as versatile Brønsted acid sites of amorphous aluminosilicate surfaces. *Angewandte Chemie - International Edition*, **2009**, 48, 2891-3	16.4	104
56	Insights into the Geometry, Stability and Vibrational Properties of OH Groups on γ-Al2O3, TiO2-Anatase and MgO from DFT Calculations. *Topics in Catalysis*, **2009**, 52, 1005-1016	2.3	29
55	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		15
54	Topological Analysis of the Interactions between Organic Molecules and Co(Ni)MoS Catalytic Active Phases. *Journal of Chemical Theory and Computation*, **2009**, 5, 580-93	6.4	10
53	Theoretical Unraveling of Selective 1-Butene Oligomerization Catalyzed by Iron Bis(arylimino)pyridine. *Organometallics*, **2009**, 28, 5358-5367	3.8	68
52	Growth of boehmite particles in the presence of xylitol: morphology oriented by the nest effect of hydrogen bonding. *Physical Chemistry Chemical Physics*, **2009**, 11, 11310-23	3.6	50
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	7.3	60
50	A DFT Chemical Descriptor to Predict the Selectivity in α-Olefins in the Catalytic Metallacyclic Oligomerization Reaction of Ethylene According to the (Hemi)labile Ligand Coordinating to Titanium. *Organometallics*, **2008**, 27, 4864-4872	3.8	22
49	Atomic scale insights on chlorinated gamma-alumina surfaces. *Journal of the American Chemical Society*, **2008**, 130, 11030-9	16.4	50
48	Evidence for the Iron(III) Oxidation State in Bis(imino)pyridine Catalysts. A Density Functional Theory Study. *Organometallics*, **2008**, 27, 3368-3377	3.8	35
47	First principles surface thermodynamics of industrial supported catalysts in working conditions. *Journal of Physics Condensed Matter*, **2008**, 20, 064235	1.8	17

46	Thermodynamic Properties of Trialkali (Li, Na, K) Hexa-alanates: A Combined DFT and Experimental Study. *Journal of Physical Chemistry C*, **2008**, 112, 18598-18607	3.8	15
45	Adsorption of NO on Pd-Exchanged Mordenite: Ab Initio DFT Modeling. *Journal of Physical Chemistry C*, **2008**, 112, 12349-12362	3.8	11
44	Optimal promoter edge decoration of CoMoS catalysts: A combined theoretical and experimental study. *Catalysis Today*, **2008**, 130, 149-159	5.3	164
43	Microkinetic interpretation of HDS/HYDO selectivity of the transformation of a model FCC gasoline over transition metal sulfides. *Catalysis Today*, **2008**, 130, 221-230	5.3	34
42	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	5.3	129
41	Aging of Co(Ni)MoP/Al2O3 catalysts in working state. *Catalysis Today*, **2008**, 130, 97-108	5.3	67
40	Predictive approach for the design of improved HDT catalysts: Alumina supported (Ni, Co) promoted Mo1WxS2 active phases. *Applied Catalysis A: General*, **2007**, 322, 92-97	5.1	70
39	Understanding and predicting improved sulfide catalysts: Insights from first principles modeling. *Applied Catalysis A: General*, **2007**, 322, 76-91	5.1	117
38	Edge wetting effects of Al2O3 and anatase-TiO2 supports by MoS2 and CoMoS active phases: A DFT study. *Journal of Catalysis*, **2007**, 246, 325-343	7.3	80
37	Interplay between molecular adsorption and metalsupport interaction for small supported metal clusters: CO and C2H4 adsorption on Pd4/Al2O3. *Journal of Catalysis*, **2007**, 247, 339-355	7.3	73
36	Transformation of a model FCC gasoline olefin over transition monometallic sulfide catalysts. *Journal of Catalysis*, **2007**, 248, 111-119	7.3	33
35	Nucleation of Pdn (n=15) clusters and wetting of Pd particles on Al2O3 surfaces: A density functional theory study. *Physical Review B*, **2007**, 75,	3.3	76
34	Quantum chemical and vibrational investigation of sodium exchanged gamma-alumina surfaces. *Physical Chemistry Chemical Physics*, **2007**, 9, 2577-82	3.6	23
33	Influence of the hydroxylation of gamma-Al2O3 surfaces on the stability and diffusion of single Pd atoms: a DFT study. *Journal of Physical Chemistry B*, **2006**, 110, 1759-67	3.4	84
32	Comment on "Examination of spinel and nonspinel structural models for gamma-Al2O3 by DFT and Rietveld refinement simulations". *Journal of Physical Chemistry B*, **2006**, 110, 20719-20; author reply 20724-6	3.4	39
31	Dual Effect of H2S on Volcano Curves in Hydrotreating Sulfide Catalysis. *Oil and Gas Science and Technology*, **2006**, 61, 515-525	1.9	22
30	A density functional theory comparison of anatase (TiO2)- and Al2O3-supported MoS2 catalysts. *Journal of Catalysis*, **2005**, 232, 161-178	7.3	85
29	DFT makes the morphologies of anatase-TiO2 nanoparticles visible to IR spectroscopy. *Journal of Catalysis*, **2005**, 236, 245-250	7.3	56

28	THERMIDOR: A new model for combined simulation of operations and optimization of catalysts in residues hydroprocessing units. *Catalysis Today*, **2005**, 109, 135-153	5.3	32
27	Effect of confinement on the selectivity of hydrocracking. *Journal of Catalysis*, **2004**, 221, 500-509	7.3	31
26	Use of DFT to achieve a rational understanding of acidBasic properties of alumina surfaces. *Journal of Catalysis*, **2004**, 226, 54-68	7.3	721
25	Effects of PH2O, PH2S, PH2 on the surface properties of anatase?TiO2 and ?-Al2O3: a DFT study. *Journal of Catalysis*, **2004**, 226, 260-272	7.3	62
24	Effects of morphology on surface hydroxyl concentration: a DFT comparison of anatase TiO2 and alumina catalytic supports. *Journal of Catalysis*, **2004**, 222, 152-166	7.3	266
23	Effects of zeolite pore sizes on the mechanism and selectivity of ´xylene´disproportionation DFT study. *Journal of Catalysis*, **2004**, 222, 323-337	7.3	29
22	Kinetic interpretation of catalytic activity patterns based on theoretical chemical descriptors. *Journal of Catalysis*, **2003**, 216, 63-72	7.3	146
21	New insights into parameters controlling the selectivity in hydrocracking reactions. *Journal of Catalysis*, **2003**, 217, 376-387	7.3	54
20	Adsorption of Unsaturated Hydrocarbons on Pd(111) and Pt(111): A DFT Study. *Journal of Physical Chemistry B*, **2003**, 107, 12287-12295	3.4	129
19	Hemilabile Ligand Induced Selectivity: a DFT Study on Ethylene Trimerization Catalyzed by Titanium Complexes. *Organometallics*, **2003**, 22, 3404-3413	3.8	105
18	Periodic trends in hydrodesulfurization: in support of the Sabatier principle. *Applied Catalysis A: General*, **2002**, 227, 83-96	5.1	161
17	Shape and Edge Sites Modifications of MoS2 Catalytic Nanoparticles Induced by Working Conditions: A Theoretical Study. *Journal of Catalysis*, **2002**, 207, 76-87	7.3	285
16	Promoter Sensitive Shapes of Co(Ni)MoS Nanocatalysts in Sulfo-Reductive Conditions. *Journal of Catalysis*, **2002**, 212, 33-38	7.3	144
15	Hydroxyl Groups on Alumina Surfaces: A DFT Study. *Journal of Catalysis*, **2002**, 211, 1-5	7.3	295
14	Structure and Stability of Aluminum Hydroxides:´ A Theoretical Study. *Journal of Physical Chemistry B*, **2002**, 106, 5155-5162	3.4	209
13	The Origin of the C7-Hydroconversion Selectivities on Y, ZSM-22, ZSM-23, and EU-1 Zeolites. *Journal of Catalysis*, **2001**, 197, 98-112	7.3	85
12	Morphology and Surface Properties of Boehmite (AlOOH): A Density Functional Theory Study. *Journal of Catalysis*, **2001**, 201, 236-246	7.3	183
11	Theoretical Study of the Dehydration Process of Boehmite to Alumina. *Journal of Physical Chemistry B*, **2001**, 105, 5121-5130	3.4	362

10	Ab Initio Study of the H2–H2S/MoS2 Gas–Solid Interface: The Nature of the Catalytically Active Sites. *Journal of Catalysis*, **2000**, 189, 129-146	7.3	292
9	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	7.3	266
8	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 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	5.3	128
7	Structural and electronic properties of the MoS2(101 0) edge-surface. *Surface Science*, **1998**, 407, 237-250	1.8	92
6	Adsorption of Thiophene on the Catalytically Active Surface of MoS2: An Ab Initio Local-Density-Functional Study. *Physical Review Letters*, **1998**, 80, 1481-1484	7.4	114
5	Ab initiodensity functional studies of transition-metal sulphides: II. Electronic structure. *Journal of Physics Condensed Matter*, **1997**, 9, 11107-11140	1.8	92
4	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	106
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*,1068-1081	13.1	2
2	Thermokinetic and Spectroscopic Mapping of Carbon Monoxide Adsorption on Highly Dispersed Pt/γ-Al2O3. *ACS Catalysis*,13280-13293	13.1	1
1	Evidence for H2-Induced Ductility in a Pt/Al2O3 Catalyst. *ACS Catalysis*,5979-5989	13.1	0