

Philippe Sautet - Publications in refereed international journals From 1987 to December 2016

- 1) P. Sautet, O. Eisenstein, K.M. Nicholas "Theoretical analysis of the addition of nucleophiles to (h₄-diene) ML_n complexes".
Organometallics, 6, 1850 (1987).
- 2) L. Salem, X. Chapuisat, G. Segal, P.C. Hiberty, C. Minot, C. Leforestier and P. Sautet "Chirality forces".
Journal of the American Chemical Society, 109, 2887 (1987).
- 3) P. Sautet, O. Eisenstein and E. Canadell "Electronic structure and delocalization in oligomeric and polymeric dicobalthexacarbonyl-acetylene complexes".
New journal of Chemistry, 11, 797 (1987).
- 4) P. Sautet and C. Joachim "Switching ability of a 3 level tight-binding system : the isolated and embedded case".
Journal of Physics C 21, 3939 (1988).
- 5) P. Sautet and C. Joachim "Electronic transmission coefficient for the single-impurity problem in the Scattering-matrix approach".
Physical Review B 38, 12238 (1988).
- 6) P. Sautet and C. Joachim "Electronic interference produced by a benzene embedded in a polyacetylene chain".
Chemical Physics letters 153, 511 (1988).
- 7) P. Sautet, O. Eisenstein and E. Canadell "The electronic transmission coefficient as a tool for the analysis of the effect of impurities and defects on the electronic structure of polymers".
Chemistry of Materials, 1, 225 (1989).
- 8) P. Sautet and C. Joachim "The Sixl-Higelin salicylideneaniline molecular switch revisited".
Chemical Physics, 135, 99 (1989).
- 9) R.J. Cave, E.R. Davidson, P. Sautet, E. Canadell and O. Eisenstein "A theoretical Study of Models for X₂Y₂ Zintl Ions".
Journal of the American Chemical Society, 111, 8105 (1989).
- 10) P. Sautet and C. Joachim "Calculation of the benzene on Rhodium STM images by the ESQC technique".
Chemical Physics Letters, 185, 23 (1991).
- 11) P. Sautet and J.F. Paul "Low Temperature Adsorption of Ethylene and Butadiene on Platinum and Palladium surfaces: a Theoretical Study of the diσ/π Competition".
Catalysis Letters, 9, 245 (1991).
- 12) F. Delbecq and P. Sautet "η¹ versus η² coordination of aldehydes and ketones in organometallic complexes. A semi-empirical study".
Journal of the American Chemical Society, 114, 2446 (1992).

- 13) P. Sautet and C. Joachim "Interpretation of large molecular adsorbate STM images: copper-phthalocyanine on copper"
Surface Science, 271, 387 (1992).
- 14) P. Sautet and C. Joachim "Are Electronic Interference Effects Important for STM Imaging of Substrates and Adsorbates? A theoretical Analysis"
Ultramicroscopy, 42-44, 115 (1992).
- 15) J.C. Dunphy, D.F. Ogletree, M.B. Salmeron, P. Sautet, M.-L. Bocquet and C. Joachim "Tip Dependent Contrast in STM Imaging of Adsorbed Sulfur Layers: Theory and Experiment"
Ultramicroscopy, 42-44, 490 (1992).
- 16) R. Orlando, C. Pisani, E. Ruiz and P. Sautet "Ab initio study of the bare and hydrated (001) surface of tetragonal zirconia"
Surface Science, 275, 482 (1992).
- 17) P. Sautet, C. Joachim, M.-L. Bocquet, M. Salmeron "STM image calculations for adsorbate recognition"; Article invité
Annales de Chimie - Sciences des matériaux, 17, 217 (1992).
- 18) C. Joachim, P. Sautet and P. Lagier "The tip apex structure of the Eigler atomic switch"
Europhysics Letters, 20, 697 (1992).
- 19) M. Dessolin, O. Eisenstein, M. Golfier, T. Prangé and P. Sautet "A Double Ionic Mechanism for the Chapman-like Rearrangement of Imino-ethers to N-Alkylamides, in the Solid State or in the Melt. Theoretical and Experimental Evidence"
Journal of the Chemical Society, Chemical Communications, p132 (1992)
- 20) J.C. Dunphy, C. Knight, P. Sautet, D.F. Ogletree, G.A. Somorjai and M.B. Salmeron "The influence of Sulfur adsorption on the step structure of vicinal Mo(100): a LEED and STM study"
Surface Science, 280, 313 (1993)
- 21) F. Delbecq and P. Sautet "Low temperature adsorption of formaldehyde on a Pt(111) surface: A theoretical study"
Langmuir, 9, 197 (1993)
- 22) X. Bouju, C. Joachim, C. Girard and P. Sautet "Moving and imaging Xe atoms on a Cu(110) surface with the tip of an STM: a theoretical study"
Physical Review B, 47, 7454 (1993)
- 23) J.C. Dunphy, P. Sautet, D.F. Ogletree; O. Dabbousi and M.B. Salmeron "Scanning Tunneling Microscopy Study of the Surface Diffusion of Sulfur on Re(0001)"
Physical Review B, 47, 2320 (1993)
- 24) C. Girard, C. Joachim, C. Chavy and P. Sautet "The electric field under a STM tip apex: Implications for adsorbate manipulation"
Surface Science, 282, 400 (1993)

- 25) J.C. Dunphy, P. Sautet, D.F. Ogletree and M.B. Salmeron "Application of STM to study adatom diffusion and lateral interactions: Sulfur on Re(0001) at low coverage"
Journal of Vacuum Science and Technology, A11, 2145-2152(1993)
- 26) J.C. Dunphy, P. Sautet, D.F. Ogletree and M.B. Salmeron "Investigation of the Structures of Sulfur on Mo(100) by STM"
Journal of Vacuum Science and Technology, A11, 1975-1982(1993)
- 27) P. Sautet, J. Dunphy, D.F. Ogletree and M. Salmeron "The role of electronic interferences in determining the appearance of STM images; application to the S(2x2)/Re(0001) system"
Surface Science, 295, 347-352 (1993)
- 28) F. Delbecq and P. Sautet "Adsorption of Aldehydes and Ketones on Platinum and Palladium: Influence of Steps, Open faces and metal nature. A theoretical study"
Surface Science, 295, 353-373 (1993)
- 29) F. Babou, B. Bigot, P. Sautet "The super-acidity of sulfated zirconia: an ab-initio quantum mechanical study"
Journal of Physical Chemistry, 97, 11501-11509 (1993)
- 30) F.J. Cadete Santos Aires, P. Sautet, G. Fuchs, J.L. Rousset and P. Melinon "Model catalysts obtained by cluster deposition of Palladium onto HOPG. TEM and STM characterisation"
Microscopy, Microanalysis, Microstructures, 4, 441-452 (1993).
- 31) M. Salmeron, G. Neubauer, A. Foch, M. Tomitori, D.F. Ogletree and P. Sautet "Viscoelastic and Electrical Properties of Alkylthiol Monolayers on Au(111) Films"
Langmuir, 9, 3600-3611 (1993).
- 32) P. Sautet and M.-L. Bocquet "A theoretical analysis of the site dependence of the shape of a molecule in STM images"
Surface Science Letters, 304, L445-L450 (1994).
- 33) B.J. McIntyre, P. Sautet, J.C. Dunphy, M. Salmeron and G.A. Somorjai "STM tip-dependent image contrast of S/Pt(111) by controlled atom transfer"
Journal of Vacuum Science and Technology, B12, 1751-1753 (1994).
- 34) P. Sautet, J.C. Dunphy, D.F. Ogletree, C. Joachim and M. Salmeron "Imaging a p(2x2) layer of sulfur on Re(0001) with the scanning tunneling microscope: an experimental and theoretical study of the effect of adsorption site and tip structure"
Surface Science, 315, 127-142 (1994)
- 35) F.J. Cadete Santos Aires, P. Sautet, J.L. Rousset, P. Mélinon and G. Fuchs "An STM and TEM study of palladium particles generated by cluster-beam deposition onto HOPG"
J. Vac. Sci. Technol., B12, 1776-1779 (1994)
- 36) A. Barbieri, D. Jentz, N. Materer, G. Held, J. Dunphy, D.F. Ogletree, P. Sautet, M. Salmeron, M.A. Van Hove and G.A. Somorjai "Surface crystallography of Re(0001)-(2x2)-S and Re(0001)-(2√3x2√3)R30°-6S: a combined LEED and STM study"

Surf. Sci., 312, 10-20 (1994)

37) F. Delbecq and P. Sautet "The effect of substituents on the adsorption of alkenes on (111) Pt and Pd surfaces: a theoretical study"
Catal. Lett. 28, 89-98 (1994)

38) J.-F. Paul and P. Sautet "The influence of the surface atom metallic coordination in the adsorption of ethylene on a Platinum surface: a theoretical study"
J. Phys. Chem 98, 10906-10912 (1994).

39) F. Delbecq and P. Sautet "Competitive C=C and C=O adsorption of α - β unsaturated aldehydes on Pt and Pd surfaces in relation with the selectivity of hydrogenation reactions: a theoretical approach"
J. Catal 152, 217-236 (1995).

40) F. Frechard and P. Sautet "Hartree-Fock ab-initio study of the geometric and electronic structure of RuS₂ and its (100) and (111) surfaces"
Surface Science 336, 149 (1995)

41) J.C. Dunphy, P. Sautet, D.F. Ogletree and M. Salmeron "Approach to surface determination with the scanning tunneling microscope: Multiple-gap imaging and electron-scattering quantum-chemistry theory"
Physical Review B52, 11446-11456 (1995)

42) P. Sautet and M.-L. Bocquet "Imaging molecules with the scanning tunneling microscope: a theoretical interpretation of benzene on platinum", *article invité*
Israeli Journal of Chemistry, 36, 63 (1996).

43) P. Sautet and M.L. Bocquet "The shape of a molecular adsorbate with the STM: a theoretical study of benzene on Pt(111)"
Physical Review B 53, 4910 (1996)

44) J.-F. Paul and P. Sautet "Density-functional periodic study of the adsorption of hydrogen on a Pd(111) surface"
Physical Review B 53, 8015 (1996)

45) M.-L. Bocquet and P. Sautet "STM and Chemistry: a qualitative Molecular Orbital understanding of the image of CO on a Pt surface"
Surface Science 360, 128-136 (1996)

46) J.F. Paul and P. Sautet "Comparison of the nature of the Hydrogen-Metal bond on Pd(111) and Ni(111) by a periodic density functional method"
Surface Science 356, L403-406 (1996)

47) A. Papakondylis and P. Sautet "Ab-initio study of the structure of α -MoO₃ solid and study of the adsorption of H₂O and CO molecules on its (100) surface"
J. Phys. Chem., 100, 10681-10688 (1996)

- 48) P. Sautet, J.C. Dunphy and M. Salmeron, "The origin of STM contrast differences for inequivalent S atoms on a Mo(100) surface"
Surface Science, 364, 335-344 (1996)
- 49) F. Delbecq and P. Sautet "Electronic and chemical properties of the Pt₈₀Fe₂₀(111) alloy surface: a theoretical study of the adsorption of atomic H, CO and unsaturated molecules"
J. Catal., 164, 152 (1996)
- 50) H. Galloway, P. Sautet and M. Salmeron "Structure and contrast in Scanning Tunneling Microscopy of Oxides: FeO Monolayer on Pt(111)"
Phys. Rev. B rapid, 54, R11145-R11148 (1996)
- 51) A. Altibelli, C. Joachim and P. Sautet "Interpretation of STM images: the MoS₂ surface"
Surface Science, 367, 209 (1996)
- 52) P. Sautet "Atomic adsorbate identification with the STM: a theoretical approach"
Surface Science, 374, 406-417 (1997)
- 53) W. Dong, V. Ledentu and P. Sautet "A theoretical study of the H-induced reconstruction of the Pd(110) surface"
Surface Science, 377-379, 56-61 (1997)
- 54) P. Sautet "Images of adsorbates with the Scanning Tunneling Microscope: Theoretical approaches to the contrast mechanism"
Chem. Rev. 97, 1097-1116 (1997)
- 55) P. Hermann, D. Simon, P. Sautet, B. Bigot "A theoretical study of butadiene adsorption on the Pd-Ni bimetallic system"
J. Catal., 167, 33-42 (1997)
- 56) F. Frechard and P. Sautet "RuS₂ (111) surfaces: theoretical study of the various terminations and their interaction with H₂"
J. Catal., 170, 402-410 (1997)
- 57) F. Frechard and P. Sautet "Chemisorption of H₂ and H₂S on the (100) surface of RuS₂: an ab-initio theoretical study"
Surf. Sci., 389, 131- 146 (1997)
- 58) F. Vigné-Maeder and P. Sautet "Theoretical study of hydroxylated and dehydroxylated surfaces of a cristobalite model of Silica"
J. Phys. Chem. B, 101, 8195-8201 (1997)
- 59) F. Delbecq, L. Vérité and P. Sautet "Electronic structure and magnetism of ordered palladium-manganese and palladium-chromium alloys"
Chem. Mat., 9, 3072-3082 (1997)
- 60) J. Cerda, M.A. Van Hove, P. Sautet and M. Salmeron "Efficient method for the simulation of STM images: I. Generalized Green Function formalism"
Phys. Rev. B56, 15885-15899 (1997)

- 61) J. Cerda, A. Yoon, M.A. Van Hove, P. Sautet, M. Salmeron, G.A. Somorjai "Efficient method for the simulation of STM images: II. Application to clean Rh(111) and Rh(111)+c(4x2)-2S"
Phys. Rev. B56, 15900-15918 (1997)
- 62) J.F. Paul, P. Sautet "Chemisorption and transformation of CH_x fragments (x=0-3) on a Pd(111) surface: a periodic density functional study"
J. Phys. Chem. B 102, 1578-1585 (1998)
- 63) M. Bernard, V. Guiral, F. Delbecq, F. Fache, P. Sautet, M. Lemaire "Structure of the diamine-Rh(I) precursor in the asymmetric hydride transfer reduction of ketones: a theoretical and experimental approach"
J. Am. Chem. Soc. 120, 1441-1446 (1998)
- 64) J. Cerda, M.A. Van Hove, P. Sautet and M. Salmeron "The role of surface relaxations in determining the STM images of sulfur adatoms and clusters on Re(0001): theory vs. experiment"
Surf. Sci. 409, 145-159 (1998)
- 65) D. Loffreda, D. Simon, P. Sautet "Molecular and dissociative chemisorption of NO on palladium and rhodium (100) and (111) surfaces: a density-functional periodic study"
J. Chem. Phys., 108, 6447-6457 (1998)
- 66) V. Ledentu, W. Dong, P. Sautet, G. Kresse, J. Hafner "H-induced reconstructions of Pd(110)"
Phys. Rev. B, 57, 12482-12491 (1998)
- 67) D.E. Bürgler, P. Hermann, S. Corbel, C.M. Schmidt, D.M. Schaller, P. Sautet, A. Baratoff, H.-J. Güntherodt "Imaging Ga tetramers on Ag(001) by scanning tunneling microscopy: theory and experiment "
Phys. Rev. B, 57, 10035-10043 (1998)
- 68) F. Touchard, M. Bernard, F. Fache, F. Delbecq, V. Guiral, P. Sautet, M. Lemaire "Optically active nitrogen ligands in asymmetric catalysis. Mechanistic study and effect of the nitrogen substitution in the enantioselective transfer hydrogenation of acetophenone"
J. Organomet. Chem. 567, 133-136 (1998)
- 69) J.C. Dunphy, M. Rose, S. Behler, D.F. Ogletree, M. Salmeron, P. Sautet "Acetylene structure and dynamics on Pd(111) "
Phys. Rev. B, 57, R12705-12708 (1998)
- 70) V. Ledentu, W. Dong, P. Sautet
"Ab initio study of the dissociative adsorption of H₂ on the Pd(110) surface"
Surf. Sci. 412-413, 518-526 (1998).
- 71) D. Loffreda, D. Simon, P. Sautet
"Vibrational frequency and chemisorption site: a DFT-periodic study of NO on Pd(111) and Rh(111) surfaces"
Chem. Phys. Lett. 291, 15 (1998)

- 72) M.-L. Bocquet, P. Sautet
"Molecular transparency and contrast with the STM: a theoretical comparison of carbon monoxide and ethylene"
Surf. Sci. 415, 148-155 (1998).
- 73) W.Dong, V.Ledentu, Ph.Sautet, A. Eichler and J. Hafner
"Hydrogen adsorption on palladium: a comparative study of different surfaces"
Surf. Sci. 411, 123-136 (1998).
- 74) M.O. Pedersen, M.-L. Bocquet, P. Sautet, E. Laegsgaard, I. Stensgaard, F. Besenbacher
"CO on Pt(111): binding site assignment from the interplay between measured and calculated images"
Chem. Phys. Lett. 299, 403 - 409 (1999)
- 75) F. Delbecq, P. Sautet
"Density Functional periodic study of CO adsorption on the Pd₃Mn(100) alloy surface: comparison with Pd(100)"
Phys. Rev. B 59, 5142-5153 (1999)
- 76) D. Loffreda, D. Simon, P. Sautet
"Dependence of stretching frequency on surface coverage and adsorbate-adsorbate interactions: a Density-Functional Theory approach of CO on Pd(111)"
Surf. Sci. 425, 68-80 (1999)
- 77) Interplay between magnetism and chemisorption: a theoretical study of CO and NO adsorption on a Pd₃Mn alloy surface
F. Delbecq, P. Sautet
Chem. Phys. Lett. 302, 91-97 (1999)
- 78) M.-L. Bocquet, J. Cerda and P. Sautet
"Transformation of molecular oxygen on a platinum surface: a theoretical calculation of STM images"
Physical Review B, 59, 15437-15445 (1999)
- 79) S. Corbel, J. Cerda, P. Sautet
"Ab initio calculations of scanning tunneling microscopy images within a scattering formalism"
Physical Review B, 60, 1989-1999 (1999)
- 80) A. Milenkovic, E. Schulz, V. Meille, D. Loffreda, M. Forissier, M. Vrinat, P. Sautet and M. Lemaire
"Selective Elimination of Alkyldibenzothiophene from Gas Oil by Formation of insoluble Charge-Transfer complexes"
Energy & Fuels 13, 881 - 887 (1999)
- 81) M.E. Grillo, V. Smelyanski, P. Sautet, and J. Hafner
"Density Functional Study of the Structural and Electronic Properties of RuS₂(111): I. Bare Surfaces"
Surf. Sci. 439, 163-172 (1999)

- 82) F. Delbecq, P. Sautet "NO adsorption on a magnetic alloy surface: a DF periodic study of Pd₃Mn(100) compared with Pd(100)"
Surf. Sci. 442, 338-348 (1999)
- 83) V. Ledentu , W. Dong, P. Sautet
"Heterogeneous catalysis through subsurface sites"
J. Am. Chem. Soc. 122, 1796-1801 (2000)
- 84) V. Guiral, F. Delbecq, P. Sautet
"A theoretical study of the mechanism of the carbonyls reduction by a rhodium(I) hydride complex. 1. The two-step Mechanism"
Organometallics, 19, 1589 - 1598 (2000)
- 85) P. Sautet, M.K. Rose, J.C. Dunphy, S. Behler, and M. Salmeron
Adsorption and energetics of isolated CO molecules on Pd(111)
Surface Science, 453, 25-31 (2000)
- 86) P. Sautet
"Theoretical chemistry as a tool for interpreting catalysts selectivities"
Topics in Catalysis, 13, 213-219 (2000)
- 87) C.I. Carlisle, D.A. King, M.-L. Bocquet, J. Cerda, P. Sautet
"Imaging the surface and the interface atoms of an oxide film on Ag(111) by scanning tunneling microscopy : experiment and theory "
Physical Review Letters, 84, 3899 – 3902 (2000)
- 88) M.E. Grillo , P. Sautet
"Density Functional Study of the Structural and Electronic Properties of RuS₂(111): II. Hydrogenated Surfaces"
Surf. Sci. 457, 285-293 (2000)
- 89) M. Bernard, F. Delbecq, P. Sautet, F. Fache, M. Lemaire
"Catalytic Asymmetric Hydrogen transfer Reduction of Ketones with Rhodium and chiral Diamine Ligands : approach of the Active Species Structure by DFT Calculations "
Organometallics 19, 5715-5722 (2000)
- 90) J.-S. Filhol, D. Simon, P. Sautet
"Stress induced nanostructure in a Pd monolayer on Ni(110) : a first-principles theoretical study"
Surf. Sci. 472, L139-L144 (2001)
- 91) A.J. Renouprez, J.F. Trillat, G. Bergeret, P. Delichère, J.L. Rousset, J. Massardier, D. Loffreda, D. Simon, F. Delbecq, and P. Sautet
Pd-Mn Silica Supported Catalysts : 2. Description of the Catalytic Sites and Surface Properties for the CO and NO Chemisorption
J. Catal. 198, 243-255 (2001)
- 92) D. Loffreda, F Delbecq, D. Simon, P. Sautet

Alloying effects on N-O stretching frequency: A DFT study of the adsorption of NO on Pd₃Mn(100) and (111) surfaces

J. Phys. Chem B, 105, 3027-3033 (2001)

93) M. Bernard, F. Delbecq, F. Fache, P. Sautet and M. Lemaire

Dithiourea ligands in Rhodium-Catalyzed Hydride-Transfer Reduction of Ketones – a Theoretical and experimental approach

Eur. J. Org. Chem 2001, 1589-1596

94) V. Guiral, F. Delbecq and P. Sautet

Origin of the enantioselectivity in the hydrogen Transfer reduction of carbonyls by a rhodium(I) complex : a theoretical study

Organomet. 20, 2207-2214 (2001)

95) L. A. M. M. Barbosa and P. Sautet

Stability of Chiral Domains produced by adsorption of Tartaric acid isomers on the Cu(110) surface : a periodic density functional study

J. Am. Chem. Soc. 123, 6639-6648 (2001)

96) M.E. Grillo and P. Sautet

On the nature of RuS₂ HDS active sites : insight from ab initio theory

J. Mol. Catal. A : Chemical 174, 239-244 (2001)

97) D. Loffreda, F. Delbecq, D. Simon, P. Sautet

Breaking the NO bond on Rh, Pd, and Pd₃Mn alloy (100) surfaces : A quantum chemical comparison of reaction paths

J. Chem. Phys., 115, 8101-8111 (2001)

98) J.-S. Filhol, D. Simon, P. Sautet

Surface phase stability for Pd deposits on Ni(110): A first-principles theoretical study

Phys. Rev. B, 64, 085412 (2001)

99) H.F. Busnengo, W. Dong, P. Sautet, A. Salin

Surface temperature dependence of rotational excitation of H₂ scattered from Pd(111)

Phys. Rev. Lett. 87, 127601 (2001)

100) L.A.M.M. Barbosa, D. Loffreda, P. Sautet

Chemisorption of trichloroethene on the PdCu Alloy (110) surface : a periodical density functional study

Langmuir, 18 (2002), 2625-2635

101) Y. Jugnet, J.C. Bertolini, L.A.M.M. Barbosa and P. Sautet

Vibrational identification of the surface reaction intermediates for the dehalogenation of trichloroethene on PdCu (100) alloy

Surf.Sci., 505, 153-162 (2002)

102) L.A.M.M. Barbosa and P. Sautet

Trichloroethene dechlorination reactions on the PdCu(110) alloy surface : a periodical density functional theory study of the mechanism

J. Catal., 207, 127-138 (2002)

- 103) A. Deluzet, H. Duclausaud, P. Sautet and S.A. Borshch
Electronic Structure of Diamagnetic and Paramagnetic Hexanuclear Chalcohalide Clusters of Rhenium
Inorg. Chem., 41, 2537-2542 (2002)
- 104) M. Digne, P. Sautet, P. Raybaud, H. Toulhoat, E. Artacho
Structure and stability of aluminum hydroxides: A theoretical study.
J. Phys. Chem., 106, 5155-5162 (2002)
- 105) Guillaume Poulet, Philippe Sautet, Alain Tuel
"Structure of Hydrated Microporous Aluminophosphates: Static and Molecular Dynamics Approaches of AlPO₄-34 from first Principles Calculations"
J. Phys. Chem., 106, 8599-8608 (2002)
- 106) F. Delbecq, P. Sautet
A density functional study of adsorption structures of unsaturated aldehydes on Pt(111) : a key factor for hydrogenation selectivity.
J. Catal., 211, 398-406 (2002)
- 107) M. K. Rose, T. Mitsui, J. Dunphy, A. Borg, D. F. Ogletree, M. Salmeron and P. Sautet,
Ordered structures of CO on Pd(111) studied by STM
Surface Science, 512, 48-60 (2002)
- 108) M. Digne, P. Sautet, P. Raybaud, P. Euzen and H. Toulhoat
Hydroxyl groups on γ -Alumina Surface : a DFT Study
J. Catal., Priority Communication, 211, 1-5 (2002)
- 109) J.-S. Filhol, M.C. Saint-Lager, M. De Santis, D. Simon, R. Baudoing-Savois, J.C. Bertolini and P. Sautet
Highly Strained Structure of a Four-Layer Deposit of Pd on Ni(110) : A coupled Theoretical and Experimental Study
Phys. Rev. Lett., 89, 146106 (2002)
- 110) Robin Hirschl, Françoise Delbecq, Philippe Sautet, J. Hafner
Pt₈₀Fe₂₀ surface from first principles: Electronic structure and adsorption of CO and atomic H
Phys. Rev. B, 66, 155438 (2002)
- 111) D. Loffreda, D. Simon and P. Sautet
Structure Sensitivity for NO Dissociation on Palladium and Rhodium Surfaces
J. Catal. 213, 211-225 (2003)
- 112) J.S. Filhol, D. Simon, P. Sautet
Ethylene adsorption and co-adsorption with H on Pd(110) from first principles
J. Phys. Chem. B 107, 1604-1615 (2003)
- 113) L.A.M.M. Barbosa and P. Sautet
Pyroglutamic acid as a chiral auxiliary in the diastereoselective hydrogenation of disubstituted aromatic rings on Rh(111) : a periodic density functional theory approach
Journal of Catalysis, 217, 23 (2003)

- 114) A. Michaelides, M.-L. Bocquet, P. Sautet, A. Alavi, D.A. King
Structures and thermodynamic phase transitions for oxygen and silver oxide phases on Ag{111}
Chem. Phys. Lett., 367, 344-350 (2003)
- 115) A. Gil, A. Clotet, J.M. Ricart, G. Kresse, M. Garcia-Hernandez, Notker Rösch and Philippe Sautet
Site preference of CO chemisorbed on Pt(111) from density functional calculations
Surface Science, 530, 7187 (2003)
- 116) R. Hirschl, F. Delbecq, P. Sautet and J. Hafner
Adsorption of unsaturated aldehydes on the (111) surface of a Pt-Fe alloy catalyst from first principles
Journal of Catalysis, 217, 354-366 2003
- 117) C. Morin, D. Simon and P. Sautet
Density-Functional Study of the adsorption and vibration Spectra of Benzene Molecules on Pt(111)
J. Phys. Chem. B, 107, 2995 (2003)
- 118) M.-L. Bocquet, P. Sautet, J. Cerda, C.I. Carlisle, M.J. Webb, and D.A. King
Specific Ethene surface activation on silver oxide covered Ag(111) from the interplay of STM experiment and theory
J. Am. Chem. Soc. 125, 3119-3125 (2003)
- 119) M.-L. Bocquet, A. Michaelides, D. Loffreda, P. Sautet, A. Alavi, D. King
New insights into ethene epoxidation on two oxidized Ag(111) surfaces
J. Am. Chem. Soc. 125, 5620-5621 (2003)
- 120) M.-L. Bocquet, A. Michaelides, P. Sautet, D. King
Initial stages in the oxidation and reduction of the 4 x 4 surface oxide phase on Ag{111}: A combined density-functional theory and STM simulation
Phys. Rev. B 68, 075413 (2003)
- 121) Guillaume Poulet, Philippe Sautet, and Emilio Artacho
Comparison between plane-wave and linear-scaling localized basis sets for structural calculations of microporous molecular sieves
Phys. Rev. B 68, 075118 (2003)
- 122) G. Kresse, A. Gil, and P. Sautet
Single-electron energies for the description of CO on Pt(111)
Phys. Rev. B 68, 073401 (2003)
- 123) F. Delbecq, V. Guiral, P. Sautet
Contribution of DFT calculations to the understanding of an asymmetric reaction, the hydrogen transfer reduction of Ketones by a Rhodium(I) complex
Eur. J. Org. Chem. 2003, 2092-2097
- 124) F. Delbecq, P. Sautet

Influence of Sn additives on the selectivity of hydrogenation of α - β unsaturated aldehydes with Pt catalysts. A density functional study of molecular adsorption
J. Catal. 220, 115 (2003)

125) C. Morin, A. Eichler, R. Hirschl, P. Sautet, J. Hafner
DFT study of adsorption and dissociation of thiophene molecules on Ni(110)
Surface Science, 540, 474-490 (2003)

126) M.-L. Bocquet, P. Sautet
"Thermal excitation of CO-Pt on the (2x1) Pt {110} surface: a theoretical simulation of a variable-temperature STM contrast"
Chem. Phys. Lett. , 382, 41-47 (2003)

127) Ana Valcárcel ^{a,b}, Anna Clotet^a, Josep M. Ricart ^a, Françoise Delbecq ^{b,*}, Philippe Sautet
Comparative DFT study of the adsorption of 1,3-butadiene, 1-butene and 2-cis/trans-butenes on the Pt(111) and Pd(111) surfaces
Surface Science 549, 121-133 (2004)

128) J.-S. Filhol, D. Simon, P. Sautet
Understanding the high activity of a nanostructured catalyst obtained by a deposit of Pd on Ni : first principle calculations
J. Am. Chem. Soc. 126, 3228-3233 (2004)

129) Alexandra Milenkovic, David Loffreda, Emmanuelle Schulz, Henry Chermette, Marc Lemaire and Philippe Sautet
Charge transfer complexes between tetranitrofluorenone and polyaromatic compounds from gasoil: a combined DFT and experimental study.
Phys. Chem. Chem. Phys. 6, 1169 – 1180 (2004)

130) N.H. de Leeuw, C.J. Nelson, C.R.A. Catlow, P. Sautet and W. Dong
Density-functional theory calculations of the adsorption of Cl at perfect and defective Ag(111) surfaces
Phys. Rev. B 69, 045419 (2004)

131) C. Morin, D. Simon, P. Sautet
Chemisorption of benzene on Pt(111), Pd(111) and Rh(111) metal surfaces : a structural and vibrational comparison from first principles
J. Phys. Chem B 108, 5653-5665 (2004)

132) C.G.M. Hermse, A.P. van Bavel, A.P.J. Jansen, L.A.M.M Barbosa, P. Sautet, R.A. van Santen
Formation of chiral domains for tartaric acid on Cu(110) : a combined DFT and dynamic Monte-carlo study
J. Phys. Chem. B, 108, 11035 (2004)

133) Loffreda D, Jugnet Y, Delbecq F, Bertolini JC, Sautet P
Coverage dependent adsorption of acrolein on pt(111) from a combination of first principle theory and HREELS study
J. Phys. Chem. B, 108, 9085-9093 (2004)

- 134) M. Digne, P. Sautet, P. Raybaud, P. Euzen and H. Toulhoat
Use of DFT to achieve a rational understanding of acid–basic properties of γ -alumina surfaces
Journal of Catalysis, 226, 54-68 (2004)
- 135) L. Piccolo, D. Loffreda, F.J. Cadete Santos Aires, C. Deranlot, Y. Jugnet, P. Sautet, J.C. Bertolini
The adsorption of CO on Au(111) at elevated pressures studied by STM, RAIRS and DFT calculations
Surf. Sci., 566-569, 995-1000 (2004)
- 136) C. Morin, D. Simon, P. Sautet
Trends in the chemisorption of aromatic molecules on a Pt(111) surface : benzene, naphthalene, and anthracene from first principles calculations
J. Phys. Chem. B 108, 12084-12091 (2004)
- 137) D. Loffreda, F. Delbecq, and P. Sautet
“Adsorption thermodynamics of acrolein on Pt(111) in realistic temperature and pressure from first-principles calculations”
Chem. Phys. Letters 2005, 405, 434-439.
- 138) A. del Vitto, G. Pacchioni, F. Delbecq and P. Sautet
“Au atoms and dimers on the MgO(100) surface: a DFT study of nucleation at defects”. *J. Phys. Chem. B* 2005, 109, 8040-8048.
- 139) D. Loffreda, P. Sautet
"A First-Principles Study of CO Adsorption and Vibration on Au surfaces", *Journal of Physical Chemistry B*, 109 (2005) 9596-9603.
- 140) E. Ozensoy, C. Hess, D. Loffreda, P. Sautet, D. W. Goodman
"Formation of a High Coverage (3x3) NO phase on Pd(111) at Elevated Pressures: Interplay between Kinetic and Thermodynamic Accessibility"
Journal of Physical Chemistry B, vol. **109** (2005) 5414-5417.
- 141) A. Valcárcel, A. Clotet, J. M. Ricart, F. Delbecq, P. Sautet
“Selectivity control for the catalytic 1,3- butadiene hydrogenation on Pt(111) and Pd(111) surfaces : radical versus closed-shell intermediates.”
J. Phys. Chem. B, 2005, 109, 14175-14182.
- 142) D. Loffreda, F. Delbecq, F. Vigné and P. Sautet
“Catalytic hydrogenation of unsaturated aldehydes on Pt(111): understanding the selectivity from first-principle calculations.”
Angew. Chem. Int. Ed. 2005, 44, 5279-5282.
- 143) D. Loffreda, L. Piccolo and P. Sautet,
"Surface Restructuring Under Gas Pressure From First Principles: A Mechanism for the CO-Induced Removal of the Au(110)-(1x2) Reconstruction"
Physical Review B, vol. 71 (2005) 113414.
- 144) Poulet G, Tuel A, Sautet P

- "A combined experimental and theoretical evaluation of the structure of hydrated microporous aluminophosphate AlPO₄-18"
J. Phys. Chem. B, 109, 22939-22946 (2005)
- 145) D. Loffreda, F. Delbecq, F. Vigné and P. Sautet
"Chemo-Regioselectivity in Heterogeneous Catalysis : Competitive routes for C=O and C=C hydrogenations from a theoretical approach"
J. Am. Chem. Soc. 128, 1316-1323 (2006)
- 146) M.C. Valero, P. Raybaud, P. Sautet
Influence of the hydroxylation of gamma-Al₂O₃ surfaces on the stability and diffusion of single Pd atoms : A DFT Study"
J. Phys. Chem. B 110, 1759 (2006)
- 147) C. Morin, D. Simon, P. Sautet
"Intermediates in the hydrogenation of benzene to cyclohexene on Pt(111) and Pd(111) : a comparison from DFT calculations"
Surf. Sci. 600, 1339 (2006)
- 148) J. Joubert, P. Fleurat-Lessard, F. Delbecq, P. Sautet
"Simulating temperature programmed desorption of water on hydrated gamma-alumina from first-principles calculations"
J. Phys. Chem. B 110, 7392 (2006)
- 149) C. Popa, C. F. J. Flipse, A. P. J. Jansen, R.A. van Santen and P. Sautet
"NO structures adsorbed on Rh(111): Theoretical approach to high-coverage STM images"
Phys. Rev. B 73, Art. No. 245408 (2006)
- 150) J. Joubert, F. Delbecq, P. Sautet, E. Le roux, M. Taoufik, C. Thieuleux, F. Blanc, C. Coperet, C. Thivole-Cazat, Basset J.M.,
"Molecular understanding of alumina supported single-site catalysts by a combination of experiment and theory"
J. Am. Chem. Soc. 128, 9157 (2006).
- 151) Céline Chizallet, Guylène Costentin, Michel Che, Françoise Delbecq, and Philippe Sautet,
"Revisiting Acido-basicity of the MgO Surface by Periodic Density Functional Theory Calculations: Role of Surface Topology and Ion Coordination on Water Dissociation"
J. Phys. Chem. B 110, 15878-15886 (2006)
- 152) Mathieu Digne, Pascal Raybaud, Philippe Sautet, Bernadette Rebours and Hervé Toulhoat,
Comment on "Examination of Spinel and Nonspinel Structural Models for γ -Al₂O₃ by DFT and Rietveld Refinement Simulations"
J. Phys. Chem. B 2006, 110, 20719-20720 (2006)
- 153) J. Joubert, A. Salameh, V. Krakoviack, F. Delbecq, P. Sautet, C. Copéret and J.M. Basset
Heterolytic splitting of H₂ and CH₄ on gamma-alumina as a structural probe for defect sites
J. Phys. Chem. B 110, 23944-23950 (2006)

- 154) C. Chizallet, G. Costentin, H. Lauron-Pernot, J. M. Krafft, P. Bazin, J. Saussey, F. Delbecq, P. Sautet and M. Che
“Role of hydroxyl groups in the basic reactivity of MgO: a theoretical and experimental study”
OIL & GAS SCIENCE AND TECHNOLOGY 61 479-488 (2006)
- 155) M.C. Valero, M. Digne, P. Sautet, P. Raybaud.
“DFT study of the interaction of a single palladium atom with gamma-alumina surfaces: the role of hydroxylation”
OIL & GAS SCIENCE AND TECHNOLOGY 61 535-545 (2006)
- 156) Jan Haubrich, David Loffreda, Françoise Delbecq, Yvette Jugnet, Philippe Sautet, Aleksander Krupski, Conrad Becker, Klaus Wandelt
“Determination of the crotonaldehyde structures on Pt and PtSn surface alloys from a combined experimental and theoretical study”
Chemical Physics Letters 433, 188–192 (2006)
- 157) Manuel Corral Valero, Pascal Raybaud and Philippe Sautet
“Nucleation of Pd_n (n=1–5) clusters and wetting of Pd particles on γ -Al₂O₃ surfaces: a density functional theory study”
Physical Review B 75, Art. No. 045427 (2007)
- 158) Cédric Trolliet, Guillaume Poulet, Alain Tuel, James D. Wuest and Philippe Sautet
“A Theoretical Study of Cohesion, Structural Deformation, Inclusion, and Dynamics in Porous Hydrogen-Bonded Molecular Networks”
Journal of the American Chemical Society, 129, 3621-3626 (2007)
- 159) Céline Chizallet, Guylène Costentin, Michel Che, Françoise Delbecq, Philippe Sautet
“Infra-red characterization of hydroxyl groups on MgO: a combined periodic and cluster computational study”
Journal of the American Chemical Society, 129, 6442-5452 (2007)
- 160) Mathieu Digne, Pascal Raybaud, Philippe Sautet, Denis Guillaume, Hervé Toulhoat
“Quantum chemical and vibrational investigation of sodium exchanged gamma-alumina surfaces”
Phys. Chem. Chem. Phys, 9, 2577-2582 (2007)
- 161) Manuel Corral Valero, Pascal Raybaud and Philippe Sautet
“Interplay between molecular adsorption and metal-support interaction for small supported metal clusters: CO and C₂H₄ adsorption on Pd₄/ γ -Al₂O₃”
J. Catal. 247, 339-355 (2007)
- 162) Alain Salameh, Jérôme Joubert, Anne Baudouin, Wayne Lukens, Françoise Delbecq, Philippe Sautet, Jean Marie Basset and Christophe Copéret
“CH₃ReO₃ on γ -Al₂O₃ : Understanding Its Structure, Initiation, and Reactivity in Olefin Metathesis”
Angew. Chem. Int. Ed. 46, 3870-3873 (2007)
- 163) Jérôme Joubert, Françoise Delbecq, Chloé Thieuleux, Mostafa Taoufik, Frédéric Blanc,

- Christophe Copéret, Jean Thivolle-Cazat, Jean-Marie Basset and Philippe Sautet
“Synthesis, Characterization, and Catalytic Properties of γ -Al₂O₃-Supported Zirconium Hydrides through a Combined Use of Surface Organometallic Chemistry and Periodic Calculations”
Organometallics 26, 3329-3335 (2007)
- 164) Rafael Anez and Philippe Sautet
“Structural Transformation of (110) Ultrathin Films of Tetragonal Zirconia Induced by Polarity”
J. Phys. Chem. C, 111, 8314-8320 (2007)
- 165) S. González, D. Loffreda, P. Sautet and F. Illas,
“Theoretical study of NO dissociation on stepped Rh(221) and RhCu(221) surfaces”
J. Phys. Chem. C, 111 11376-11383 (2007)
- 166) Jérôme Joubert, Françoise Delbecq and Philippe Sautet
“Alkane metathesis by a tungsten carbyne complex grafted on gamma alumina: Is there a direct chemical role of the support ? ”
J. Catal. 251 (2007) 507-513
- 167) Céline Chizallet, Guylène Costentin, Hélène Lauron-Pernot, Michel Che, Christian Bonhomme, Jocelyne Maquet, Françoise Delbecq and Philippe Sautet
“Study of the Structure of OH Groups on MgO by 1D and 2D 1H MAS NMR Combined with DFT Cluster Calculations”
J. Phys. Chem. C, 111 18279-18287 (2007)
- 168) P. Raybaud, D. Costa, M. Corral Valero, C. Arrouvel, M. Digne, P. Sautet and H. Toulhoat
“First principles surface thermodynamics of industrial supported catalysts in working conditions”
J. Phys.: Condens. Matter 20, 064235 (2008)
- 169) Jan Haubrich, David Loffreda, Françoise Delbecq, Philippe Sautet, Yvette Jugnet, A. Krupski, Conrad Becker, Klaus Wandelt
Adsorption and Vibrations of α - β unsaturated Aldehydes on pure Pt and Pt-Sn Alloy (111) Surfaces I. Prenal
J. Phys. Chem. C 112, 3701-3718 (2008)
- 170) J. Handzlik, P. Sautet
Active sites of olefin metathesis on molybdena-alumina system: a periodic DFT study
J. Catal. 256, 1-14 (2008)
- 171) Jérôme Joubert, Françoise Delbecq, Christophe Coperet, Jean-Marie Basset and Philippe Sautet
Gamma-alumina: An active support to obtain immobilized electron poor Zr complexes
Topics in Catalysis 48, 114-119 (2008)
- 172) M. Digne, P. Raybaud, P. Sautet, D. Guillaume, H. Toulhoat
Atomic Scale Insights on Chlorinated γ -Alumina Surfaces
J. Am. Chem. Soc. 130, 11030-11039 (2008)

- 173) Detre Teschner, Zsolt Révay, János Borsodi, Michael Hävecker, Axel Knop-Gericke, Robert Schlögl, D. Milroy, S. David Jackson, Daniel Torres, Philippe Sautet
Understanding Pd Hydrogenation Catalysts: When Nature of the Reactive Molecule Controls the Nature of the Catalyst Active Phase
Angewandte Chemie 47, 9274 (2008)
- 174) Conrad Becker, Jan Haubrich, Klaus Wandelt, Françoise Delbecq, David Loffreda, and Philippe Sautet
Adsorption of simple alkenes on Pt(111) and Pt-Sn surface alloys: bond strength vs. heat of adsorption
J. Phys. Chem. C 112, 14693 (2008)
- 175) J. Handzlik, P. Sautet
Structure of Isolated Molybdenum(VI) Oxide Species on γ -Alumina: A Periodic Density Functional Theory Study
J. Phys. Chem. C 112, 14456 (2008)
- 176) Céline Chizallet, Guylène Costentin, Hélène Lauron-Pernot, Jean-Marc Krafft, Michel Che, Françoise Delbecq and Philippe Sautet
Assignment of Photoluminescence Spectra of MgO Powders: TD-DFT Cluster Calculations Combined to Experiments. Part I: Structure Effects on Dehydroxylated Surfaces
J. Phys. Chem. C 112, 16629-16637 (2008)
- 177) Céline Chizallet, Guylène Costentin, Hélène Lauron-Pernot, Jean-Marc Krafft, Michel Che, Françoise Delbecq and Philippe Sautet
Assignment of Photoluminescence Spectra of MgO Powders: TD-DFT Cluster Calculations Combined to Experiments. Part II: Hydroxylation Effects
J. Phys. Chem. C 112, 19710-10917 (2008)
- 178) Sylvian Cadars, Anne Lesage, Chris J. Pickard, Philippe Sautet, and Lyndon Emsley
Characterizing Slight Structural Disorder in Solids by Combined Solid-State NMR and First Principles Calculations
J. Phys. Chem. A 113, 902-911 (2009)
- 179) Benjamin Isare, Laurence Petit, Emmanuelle Bugnet, Régis Vincent, Laurence Lapalu, Philippe Sautet, Laurent Bouteiller
The weak help the strong: low molar mass organogelators harden bitumen
Langmuir 25, 8400-8403 (2009)
- 180) Chizallet C., Digne M., Arrouvel C., Raybaud P., Delbecq F., Costentin G., Che M., Sautet P., Toulhoat H.
Insights into the geometry, stability and vibrational properties of OH groups on γ -Al₂O₃, TiO₂-anatase and MgO from DFT calculations
Top. Catal. 52, 1005-1016, 2009.
- 181) Rafael Añez, Aníbal Sierraalta, Guillermo Martorell, Philippe Sautet
Stabilization of the (110) Tetragonal Zirconia surface by Hydroxyl Chemical Transformation
Surface Science 603, 2526-2531 (2009)

- 182) David Loffreda, Françoise Delbecq, Fabienne Vigné and Philippe Sautet
Fast Prediction of Selectivity in Heterogeneous Catalysis from extended Brønsted-Evans-Polanyi Relations: A Theoretical Insight
Angewandte Chemie International Edition, 48, 4978 (2009)
- 183) Jan Haubrich, David Loffreda, Françoise Delbecq, Philippe Sautet, A. Krupski, Conrad Becker, Klaus Wandelt
Adsorption of α - β unsaturated Aldehydes on Pt and Pt-Sn Alloy (111) Surfaces II. Crotonaldehyde
J. Phys. Chem. C 113, 13947-13967 (2009)
- 184) Laurence Petit, Laurence Lapalu, Philippe Sautet
Self-assembly of diacid molecules : a theoretical approach of molecular interactions
J. Phys. Chem. C. 113, 17566–17571 (2009)
- 185) F. Cinquini, F. Delbecq, P. Sautet
A DFT comparative study of carbon adsorption and diffusion on surface and subsurface of Ni and Ni₃Pd alloy
Phys. Chem. Chem. Phys. 11, 11546–11556 (2009)
- 186) F. Delbecq, D. Loffreda, P. Sautet
Heterogeneous Catalytic Hydrogenation: Is Double Bond/Surface Coordination Necessary?
J. Phys. Chem. Lett., 1, 323-326 (2010)
- 187) Jan Haubrich, David Loffreda, Françoise Delbecq, Philippe Sautet, Yvette Jugnet, Conrad Becker, Klaus Wandelt
Adsorption and Vibrations of α , β -Unsaturated Aldehydes on Pt(111) and Pt-Sn Alloy (111) surfaces. 3. Adsorption energy vs Adsorption Strength
J. Phys. Chem. C 114, 1073-1084 (2010)
- 188) F. Delbecq, P. Sautet
Catalysis and surface organometallic chemistry : a view from theory and simulations
Chem. Rev. 110, 1788-1806 (2010)
- 189) Detre Teschner, Janos Borsodi, Zoltan Kis, Laszlo Szentmiklosi, Zsolt Revay[‡], Axel Knop-Gericke, Robert Schlögl, Daniel Torres and Philippe Sautet
Role of hydrogen species in palladium-catalysed alkyne hydrogenation
J. Phys. Chem. C 114, 2293-2299 (2010)
- 190) Hugo Petitjean, Konstantin Tarasov, Françoise Delbecq, Philippe Sautet, Jean Marc Krafft, Philippe Bazin, Maria Cristina Paganini, Elio Giamello, Michel Che, Hélène Lauron-Pernot and Guylène Costentin
Quantitative Investigation of MgO Brønsted Basicity: DFT, IR, and Calorimetry Study of Methanol Adsorption
J. Phys. Chem. 114, 3008-3016 (2010)
- 191) P. Sautet, F. Cinquini,
Surface of Metallic Catalysts under a Pressure of Hydrocarbon Molecules: Metal or Carbide?
ChemCatChem 2, 636-639 (2010)

- 192) R. Wischert, C. Copéret, F. Delbecq, P. Sautet
Revisiting the structure of methyltrioxorhenium chemisorbed on alumina
ChemCatChem 2, 812-815 (2010)
- 193) Chao Hao Hu, Céline Chizallet, Christophe Mager-Maury, Manuel Corral-Valero, Philippe Sautet, Hervé Toulhoat and Pascal Raybaud
Modulation of Catalyst Particle Structure upon Support Hydroxylation: *ab initio* insights into Pd₁₃ and Pt₁₃ / γ -Al₂O₃
J. Catal. 274, 99-110 (2010)
- 194) F. Vigné, J. Haubrich, D. Loffreda, P. Sautet, F. Delbecq
Highly selective hydrogenation of butadiene on Pt/Sn alloy
J. Catal. 275, 129 (2010)
- 195) Xavier Rozanska, Françoise Delbecq, Philippe Sautet
Reconstruction and stability of β -cristobalite 001, 101, and 111 surfaces during dehydroxylation
PCCP 12, 14930-14940 (2010)
- 196) Emiel de Smit, Fabrizio Cinquini, Andrew M. Beale, Olga V. Safonova, Wouter van Beek, Philippe Sautet and Bert M. Weckhuysen
The Stability and Reactivity of ϵ - χ - θ Iron Carbide Catalyst Phases in Fischer-Tropsch Synthesis : Controlling μ_c
J. Am. Chem. Soc. 132, 14928 (2010)
- 197) David Coll, Françoise Delbecq, Yosslen Aray and Philippe Sautet
Stability of intermediates in the glycerol hydrogenolysis on transition metal catalysts from first principles
PCCP 13, 1448-1456 (2011)
- 198) E. Grinval; X. Rozanska; A. Baudouin; E. Berrier; F. Delbecq; P. Sautet; J.-M. Basset; F. Lefebvre
Controlled Interactions between Anhydrous Keggin type Heteropolyacids and Silica Support: Preparation and Characterization of well Defined Silica Supported Polyoxometalate Species.
J. Phys. Chem. C 114, 18516 (2010)
- 199) Marco Delgado, Catherine C. Santini, Françoise Delbecq, Raphaël Wischert, Boris Le Guennic, Géraldine Tosin, R. Spitz, Jean-Marie Basset, and Philippe Sautet
Alumina as a Simultaneous Support and Cocatalyst: Cationic Hafnium Complex evidenced by Experimental and DFT analyses
J. Phys. Chem. C 114, 19024-19034 (2010)
- 200) J. Handzlik, P. Sautet
Structure of Dimeric Molybdenum(VI) Oxide Species on γ -Alumina: A Periodic Density Functional Theory Study
J. Phys. Chem. C 114, 19406 (2010)
- 201) Christophe Mager-Maury, Gaëtan Bonnard, Céline Chizallet, Philippe Sautet and Pascal Raybaud

H₂ induced reconstruction of supported Pt clusters : metal-support interaction *versus* surface hydride

ChemCatChem 3, 200-207 (2011)

202) Slimane Laref, Yan Li, Marie-Laure Bocquet, Françoise Delbecq, Philippe Sautet, and David Loffreda "Nature of Adhesion of Condensed Organic Films on Platinum by First-Principles Simulations"

PCCP, 13, 11827-11837 (2011)

203) Emiel de Smit, Matti M. van Schooneveld, Fabrizio Cinquini, Hendrik Bluhm, Philippe Sautet, Frank M. F. de Groot and Bert M. Weckhuysen « Size Dependence of the Surface Chemistry of Iron Oxides in Reactive Gas Atmospheres »

Angewandte Chemie International Edition, 50, 1584-1588 (2011)

204) R. Wischert, C. Copéret, F. Delbecq, P. Sautet " Optimal water coverage on alumina: a key to generate Lewis acid-base pairs reactive towards the C-H bond activation of methane"

Angewandte Chemie International Edition, 50, 3202-3205 (2011)

205) R. Wischert, C. Copéret, F. Delbecq, P. Sautet, Dinitrogen: a selective probe for tri-coordinate Al "defect" sites on alumina

Chem. Comm. 47, 4890-4892, 2011

206) E. Dumont, C. Michel, P. Sautet, Unravelling Gold(I) specific action towards peptidic disulfide cleavage

Chem. Phys. Chem. 12, 2596 (2011)

207) Rodrigo Ferreira de Moraes, Philippe Sautet, David Loffreda, Alejandro A. Franco, A multiscale theoretical methodology for the calculation of electrochemical observables from ab initio data: Application to the oxygen reduction reaction in a Pt(1 1 1)-based polymer electrolyte membrane fuel cell

Electrochimica Acta 56, 10842-10856 (2011)

208) J. Garrec, P. Sautet, and P. Fleurat-Lessard Understanding the HIV-1 Protease Reactivity with DFT: What Do We Gain from Recent Functionals?

J. Phys. Chem. B 115, 8545–8558 (2011)

209) Marco Delgado, Catherine C. Santini, Françoise Delbecq, Anne Baudouin, Aimery De Mallmann, Carmello Prestipino, S. Norsic, Philippe Sautet, and Jean-Marie Basset, Characterization of Surface Hydride Hafnium Complexes on Alumina by a Combination of Experiments and DFT Calculations

J. Phys. Chem. C 115, 6757–6763 (2011)

210) Haubrich, J., Loffreda, D., Delbecq, F., Sautet, P. Jugnet, Y., Krupski, A., Becker, C., Wandelt, K.

Mechanistic and spectroscopic identification of initial reaction intermediates for prenal decomposition on a platinum model catalyst

Phys. Chem. Chem. Phys, 13, 6000-6009 (2011)

- 211) F. Auneau, Carine Michel, Françoise Delbecq, Catherine Pinel and Philippe Sautet "Unravelling the mechanism of glycerol hydrogenolysis over Rhodium catalyst through joined experimental-theoretical investigations"
Chem. Eur. J. 17, 14288-14299 (2011)
- 212) M. Harb, P. Sautet, P. Raybaud, "Origin of the enhanced visible-light absorption in N-doped bulk anatase TiO₂ from first principles calculations"
J. Phys. Chem. C 115, 19394 (2011)
- 213) Carine Michel, Florian Auneau, Françoise Delbecq, Philippe Sautet, "C-H vs. O-H bond dissociation on transition metal surface Rh(111) : a strong influence of the environment"
ACS catalysis, 1, 1430 (2011)
- 214) X. Rozanska, P. Sautet, F. Delbecq, F. Lefebvre, S. Borshch, H. Chermette, J.M. Basset, E. Grinval " Polyoxometalate grafting onto silica: stability diagrams of H₃PMo₁₂O₄₀ on (001), (101) and (111) beta-cristobalite surfaces analyzed by DFT"
Phys. Chem. Chem. Phys. **13**, 15955-15959 (2011)
- 215) Thuat T. Trinh, Xavier Rozanska, Françoise Delbecq, Philippe Sautet* "Initial step of silicate versus aluminosilicate formation in zeolite synthesis: reaction mechanism in water with a tetrapropylammonium template"
Phys. Chem. Chem. Phys. 14, 3369-3380 (2012)
- 216) R. N. Kerber A. Kermagoret, E. Callens, P. Florian, D. Massiot, A. Lesage, C. Copéret, F. Delbecq, X. Rozanska, P. Sautet* "Nature and structure of aluminum surface sites grafted on silica from a combination of high field aluminum-27 solid-state NMR spectroscopy and first principle calculations"
Journal of the American Chemical Society, 134, 6767-6775 (2012)
- 217) Marco Delgado, Françoise Delbecq, Catherine C. Santini, Frédéric Lefebvre, Sébastien Norsic, Piotr Putaj, Philippe Sautet, and Jean-Marie Basset, Evolution of Structure and of Grafting Properties of γ -Alumina with Pretreatment Temperature
J. Phys. Chem. C, 116, 834–843 (2012)
- 218) M. Armbrüster, M. Behrens, F. Cinquini, K. Föttinger, Y. Grin, A. Haghofer, B. Klötzer, A. Knop-Gericke, H. Lorenz, A. Ota, S. Penner, J. Prinz, C. Rameshan, Z. Révay, D. Rosenthal, G. Rupprechter, P.Sautet, R. Schlögl, L. Shao, L. Szentmiklósi, D. Teschner, D. Torres, R. Wagner, R. Widmer, G. Wowsnick, "How to control the selectivity of palladium-based catalysts in hydrogenation reactions: The role of subsurface chemistry"
Chem. Cat. Chem. 8, 1048-1063 (2012)
- 219) Christophe Mager-Maury, Gaëtan Bonnard, Céline Chizallet, Philippe Sautet and Pascal Raybaud, "Platinum nanoclusters stabilized on γ -alumina by chlorine used as a capping surface ligand: a density functional theory study"
ACS catalysis, 2 1346-1357 (2012)
- 220) Florian Auneau, Leila Sadr Arani, Michèle Besson, Laurent Djakovitch, Carine Michel, Françoise Delbecq, Philippe Sautet, Catherine Pinel " Heterogeneous Transformation of Glycerol to Lactic Acid"
Top. Catal. 55, 474 (2012)

- 221) A. Aloui, F. Delbecq, P. Sautet, C. De Bellefon "Further insight in the minor/major concept using hydrogen pressure effect in asymmetric hydrogenation"
Journal of Molecular Catalysis A: Chemical 363– 364, 214– 222 (2012)
- 222) R. Wischert, P. Laurent, C. Copéret, F. Delbecq, P. Sautet " γ -alumina: The Essential and Unexpected Role of Water for the Structure, Stability, and Reactivity of "Defect" Sites"
Journal of the American Chemical Society, 134, 14430-14449 (2012)
- 223) P. Raybaud, C. Chizallet, H. Toulhoat, and P. Sautet "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"
Phys. Chem. Chem. Phys. 14, 16773-16774 (2012)
- 224) Carine Michel, Florian Göttl, and Philippe Sautet "Early stages of water/hydroxyl phase generation at transition metal surfaces - synergetic adsorption and O-H bond dissociation assistance"
Phys. Chem. Chem. Phys. 14, 15286-15290 (2012)
- 225) G. Fu, X. Xu, P. Sautet "Vanadium distribution in the four component Mo-V-Te-Nb mixed oxide catalysts from first principles: how to explore the numerous configurations?"
Angewandte Chemie International Edition 51, 12854-12858 (2012)
- 226) Etienne Grau, Anne Lesage, Sébastien Norsic, Christophe Copéret, Vincent Monteil, Philippe Sautet "Tetrahydrofuran in TiCl₄/THF/MgCl₂: a Non-Innocent Ligand for Supported Ziegler-Natta Polymerization Catalysts"
ACS Catalysis 3, 52-56 (2013)
- 227) Anthony Kermagoret, Rachel Nathaniel Kerber, Matthew P. Conley, Emmanuel Callens, Pierre Florian, Dominique Massiot, Christophe Copéret*
Françoise Delbecq, Xavier Rozansk and Philippe Sautet « Triisobutylaluminum: bulkier and yet more reactive towards silica surfaces than triethyl or trimethylaluminum»
Dalton Trans 42, 12681-12687 (2013)
- 228) D. Torres, F. Cinquini and P. Sautet "Pressure and Temperature Effects on the Formation of a Pd C Surface Carbide: Insights into the Role of Pd C as a Selective Catalytic State for the Partial Hydrogenation of Acetylene"
J. Phys. Chem. C 117, 11059-11065 (2013)
- 229) T. Kerber, R. Kerber, X. Rozanska, P. Sautet, P. Fleurat-Lessard « QMX : A versatile environment for hybrid calculations applied to the grafting of Al₂Cl₃Me₃ on a silica surface »
J. Comput. Chem 34, 1155-1163 (2013)
- 230) M. Harb, P. Sautet, P. Raybaud, "Anionic or Cationic S-Doping in Bulk Anatase TiO₂: Insights on Optical Absorption from First Principles Calculations"
J. Phys. Chem. C 117, 8892-8902 (2013)
- 231) Florian Göttl, Rosa E. Bulo, Jürgen Hafner, Philippe Sautet
What Makes Copper-Exchanged SSZ-13 Zeolite Efficient at Cleaning Car Exhaust Gases?
J. Phys. Chem. Lett. 4, 2244-2249 (2013)

- 232) M. Harb, D. Masih, S. Ould-Chikj, P. Sautet, J.M. Basset and K. Takanebe, "Determination of the electronic structure and UV-Vis absorption properties of $(\text{Na}_{2-x}\text{Cu}_x)\text{Ta}_4\text{O}_{11}$ from first-principle calculations" *J. Phys. Chem. C* 117, 17277-17484 (2013)
- 233) Rosa E. Buló, Carine Michel, Paul Fleurat-Lessard, Philippe Sautet
Multiscale modeling of chemistry in water : Are we there Yet ?
J. Chem. Theo. Comput. 9, 5567-5577 (2013)
- 234) Pascal Raybaud, Céline Chizallet, Christophe Mager-Maury, Mathieu Digne, Hervé Toulhoat, Philippe Sautet, From γ -alumina to supported platinum nanoclusters in reforming conditions: 10 years of DFT modeling and beyond
J. Catal. 308, 328-340 (2013)
- 235) D. Loffreda, C. Michel, F. Delbecq, P. Sautet
Tuning catalytic reactivity on metal surfaces: Insights from DFT
J. Catal. 308, 374-385 (2013)
- 236) Kahina Aït Atmane, Carine Michel, Jean-Yves Piquemal, Philippe Sautet, Patricia Beaunier, Marion Giraud, Mickaël Sicard, Sophie Nowak, Rémi Losno, Guillaume Viau
Control of anisotropic shape of cobalt nanorods in liquid phase: from experiment to theory ... and back
Nanoscale 6, 2682 – 2692 (2014)
- 237) Jérémie Zaffran, Carine Michel, Florian Auneau, Françoise Delbecq, Philippe Sautet
Linear energy relations as predictive tools for polyalcohol catalytic reactivity
ACS Catalysis, 4, 464-468 (2014)
- 238) Anthony Kermagoret, Rachel Nathaniel Kerber, Matthew P. Conley, Emmanuel Callens, Pierre Florian, Dominique Massiot, Christophe Copéret, Françoise Delbecq, Xavier Rozanska, Philippe Sautet
Chlorodiethylaluminum supported on silica: a dinuclear aluminum surface species with bridging μ_2 -Cl-ligand as a highly efficient cocatalyst for the Ni-catalyzed dimerization of ethene
J. Catal. 313, 46-54 (2014)
- 239) F. Göttl, C. Houriez, M. Guitou, G. Chambaud and P. Sautet
The Importance of a Non-Local Description of Electron-Electron Interactions in Modeling the Dissociative Adsorption of H_2 on Cu(100)
J. Phys. Chem. C. 118, 5374-5382 (2014)
- 240) Tangui Le Bahers, Michel Rérat, Philippe Sautet
Semiconductors used in Photovoltaic and Photocatalytic devices: Assessing Fundamental Properties from DFT
J. Phys. Chem. C. 118, 5997-6008 (2014)
- 241) Florian Göttl and Philippe Sautet
Modeling the adsorption of short alkanes in SSZ-13 using the vdW-DF2 and BEEF-vdW functionals – Understanding advantages and limitations of vdW-type functionals

J. Chem. Phys. 140, 154105 (2014)

242) Federico Calle-Vallejo, José I. Martínez, Juan M. García-Lastra, Philippe Sautet and David Loffreda

Fast Prediction of Adsorption Properties for Platinum Nanocatalysts with Generalized Coordination Numbers

Angewandte Chemie International Edition 53, 8316-8319 (2014)

243) T. Jiang, F. Göttl, R.E. Bulo and P. Sautet

The Effect of Temperature on the Adsorption of Short Alkanes in the Zeolite SSZ-13 - Adapting Adsorption Isotherms to Microporous Materials

ACS Catalysis 4, 2351 (2014)

244) Federico Calle-Vallejo, Philippe Sautet, and David Loffreda

Understanding Adsorption-Induced Effects on Platinum Nanoparticles: An Energy-Decomposition Analysis

J. Phys. Chem. Lett. 5, 3120 (2014)

245) Carine Michel, Jérémie Zaffran, Joanna Matras-Michalska, Marcin Jedrzejczyk, Agnieszka M. Ruppert, Jacek Grams, and Philippe Sautet

Role of water on metal catalyst performance for ketone hydrogenation. A joint experimental and theoretical study on levulinic acid conversion into gamma-valerolactone

Chem. Comm. 50, 12450 (2014)

246) R. Wischert, P. Florian, C. Copéret, D. Massiot and P. Sautet

On the visibility of Al surface sites on gamma-alumina: a combined computational and experimental point of view

J. Phys. Chem. 118, 15292 (2014)

247) Ela Nurlaela, Samy Ould-Chikh, Moussab Harb, Silvano del Gobbo, Mimoun Aouine, Eric Puzenat, Philippe Sautet, Kazunari Domen, Jean-Marie Basset, and Kazuhiro Takanabe

Critical role of the semiconductor-electrolyte interface in photocatalytic performance for water-splitting reactions using Ta₃N₅ particles

Chem. Mater. 26, 4812 (2014)

248) Wenping Guo, Carine Michel, Renate Schwiedernoch, Raphael Wischert, Xin Xu, Philippe Sautet

Formation of acrylates from ethylene and CO₂ on Ni complexes: A mechanistic viewpoint from a hybrid DFT approach

Organomet. 33, 6369-6380 (2014)

249) Moussab Harb, Philippe Sautet, Ela Nurlaela, Pascal Raybaud, Luigi Cavallo, Kazunari Domen, Jean-Marie Basset and Kazuhiro Takanabe

Tuning the properties of visible light tantalum (oxy)nitride photocatalysts by non-stoichiometric compositions: a first principle viewpoint

Phys. Chem. Chem. Phys. 16, 20548 (2014)

250) Hugo Petitjean, Hazar Guesmi, H el ene Lauron-Pernot, Guyl ene Costentin, David Loffreda, Philippe Sautet and Fran oise Delbecq

How surface hydroxyls enhance MgO reactivity in basic catalysis: the case of MBOH conversion
ACS Catalysis, 4, 4004 (2014)

251) Sigismund Teunis Alexander George Melissen, Frédéric Labat, Philippe Sautet, Tangui Le Bahers
Electronic properties of $\text{PbX}_3\text{CH}_3\text{NH}_3$ ($\text{X}=\text{Cl}, \text{Br}, \text{I}$) compounds for photovoltaic and photocatalytic applications
Phys. Chem. Chem. Phys. 17, 2199-2209 (2015)

252) Soe Lwin, Christopher Keturakis, Jaroslaw Handzlik, Philippe Sautet, Yuanyuan Li, Anatoly I. Frenkel and Israel E. Wachs
Surface ReO_x Sites on Al_2O_3 and Their Molecular Structure–Reactivity Relationships for Olefin Metathesis
ACS Catal. 5, 1432–1444 (2015)

253) Rodrigo Ferreira de Morais,†,‡ Alejandro A. Franco,§,¶,□ Philippe Sautet,† and David Loffreda
Interplay between Reaction Mechanism and Hydroxyl Species for Water Formation on Pt(111)
ACS Catal. 5, 1068–1077 (2015)

254) Prokopis C. Andrikopoulos, Carine Michel, Sandra Chouzier, and Philippe Sautet
In Silico Screening of Iron-Oxo Catalysts for CH Bond Cleavage
ACS Catal. 5, 2490–2499 (2015)

255) Saranyan Vijayaraghavan, Willi Auwärter, David Eciija, Knud Seufert, Stefano Rusponi, Torsten Houwaart, Philippe Sautet, Marie-Laure Bocquet, Pardeep Thakur, Sebastian Stepanow, Uta Schlickum, Markus Etzkorn, Harald Brune and Johannes V. Barth
Restoring the Co Magnetic Moments at Interfacial Co-Porphyrin Arrays by Site-Selective Uptake of Iron
ACS Nano, 9, 3605–3616 (2015)

256) Torsten Houwaart, Tangui Le Bahers, Philippe Sautet, Willi Auwärter, Knud Seufert, Johannes V. Barth, Marie-Laure Bocquet
Scrutinizing individual CoTPP molecule adsorbed on coinage metal surfaces from the interplay of STM experiment and theory
Surface Science 635 108–114 (2015)

257) Rodrigo Ferreira de Morais, Alejandro A. Franco, Philippe Sautet and David Loffreda
Coverage-dependent thermodynamic analysis of the formation of water and hydrogen peroxide on a platinum model catalyst
Phys.Chem.Chem.Phys. 17, 11392 (2015)

258) A. M. Ruppert, J. Grams, M. Jedrzejczyk, J. Matras-Michalska, N. Keller, K. Ostojka, and P. Sautet
Titania-Supported Catalysts for Levulinic Acid Hydrogenation: Influence of Support and its Impact on γ -Valerolactone Yield
ChemSusChem 8, 1538 – 1547 (2015)

- 259) Stephan N. Steinmann, Carine Michel, Renate Schwiedernoch and Philippe Sautet
Impacts of electrode potentials and solvents on the electroreduction of CO₂: a comparison of theoretical approaches
Phys.Chem.Chem.Phys. 17, 13949 (2015)
- 260) Federico Calle-Vallejo*, David Loffreda, Marc T. M. Koper and Philippe Sautet*
Introducing structural sensitivity into scaling relations between adsorption energies by means of coordination numbers
Nature Chem. 2015, 7, 403-410.
- 261) Stephan N. Steinmann, Carine Michel, Renate Schwiedernoch, Jean-Sebastien Filhol, Philippe Sautet*
Modelling the HCOOH/CO₂ Electrocatalytic Reaction: When Details Are Key
ChemPhysChem 16, 2307 – 2311 (2015)
- 262) Florian Göttl, Philippe Sautet, and Ive Hermans
Can Dynamics Be Responsible for the Complex Multipipeak Infrared Spectra of NO Adsorbed to Copper(II) Sites in Zeolites?
Angew. Chem. Int. Ed. 54, 7799 –7804 (2015)
- 263) Jérémie Zaffran, Carine Michel, Françoise Delbecq, and Philippe Sautet
Trade-Off between Accuracy and Universality in Linear Energy Relations for Alcohol Dehydrogenation on Transition Metals
J. Phys. Chem. C, 119, 12988-12998 (2015)
- 264) Aleix Comas-Vives, Maxence Valla, Christophe Copéret and Philippe Sautet
Cooperativity between Al-sites Promotes H-Transfer and Carbon–Carbon Bond Formation upon Dimethylether Activation on Alumina
ACS Cent. Sci., 1, 313–319 (2015)
- 265) Federico Calle-Vallejo, Jakub Tymoczko, Viktor Colic, Quang Huy Vu, Marcus D. Pohl, Karina Morgenstern, David Loffreda, Philippe Sautet, Wolfgang Schuhmann, Aliaksandr S. Bandarenka
Finding optimal surface sites on heterogeneous catalysts by counting nearest neighbors
Science, 350, 185-189 (2015)
- 266) Rachel Nathaniel Kerber, Torsten Kerber, Xavier Rozanska, Françoise Delbecq, and Philippe Sautet
Grafting trimethylaluminum and its halogen derivatives on silica: General trends for ²⁷Al SS-NMR response from first principles calculations
Phys. Chem. Chem. Phys., 17, 26937-26945 (2015)
- 267) Sarah Gautier, Stephan N. Steinmann, Carine Michel, Paul Fleurat-Lessard, Philippe Sautet
Molecular adsorption at Pt(111). How accurate are DFT functionals?
Phys. Chem. Chem. Phys., 17, 28921-28930 (2015)
- 268) Sigismund Melissen, Tangui Le Bahers, Stephan N. Steinmann, and Philippe Sautet
The Relationship Between Carbon Nitride Structure and Exciton Binding Energies: A DFT Perspective

J. Phys. Chem C, 119, 25188-25196 (2015)

269) Manas K. Bhunia, Sigismund Melissen, Manas R. Parida, Pradip Sarawade, Jean-Marie Basset, Dalaver H. Anjum, Omar F. Mohammed, Philippe Sautet, Tangui Le Bahers, and Kazuhiro Takanabe

Dendritic Tip-on Polytriazine-Based Carbon Nitride Photocatalyst with High Hydrogen Evolution Activity

Chem. Mater., 27, 8237–8247 (2015)

270) Tarek A. Kandiel, Dalaver H. Anjum, Philippe Sautet, Tangui Le Bahers and Kazuhiro Takanabe

Electronic structure and photocatalytic activity of wurtzite Cu–Ga–S nanocrystals and their Zn substitution

J. Mater. Chem. A, 3, 8896–8904 (2015)

271) Aleix Comas-Vives, Martin Schwarzwälder, Christophe Copéret, Philippe Sautet

Carbon–Carbon Bond Formation by Activation of CH₃F on Alumina

J. Phys. Chem. C 119, 7156–7163 (2015)

272) T. Jahnke, G. Futter, A. Latz, T. Malkow, G. Papakonstantinou, G. Tsotridis, P. Schott, M. Gérard, M. Quinaud, M. Quiroga, A.A. Franco, K. Malek, F. Calle-Vallejo, R. Ferreira de Morais, T. Kerber, P. Sautet, D. Loffreda, S. Strahl, M. Serra, P. Polverino, C. Pianese, M. Mayur, W.G. Bessler, C. Kompis

Performance and degradation of Proton Exchange Membrane Fuel Cells: State of the art in modeling from atomistic to system scale

Journal of Power Sources 304, 207–233 (2016)

273) Florian Göttl, Philippe Sautet, Ive Hermans

The Impact of Finite Temperature on the Coordination of Cu Cations in the Zeolite SSZ-13

Catal. Today, 267, 41-46 (2016)

274) Agnieszka M. Ruppert, Marcin Jędrzejczyk, Olga Sneka-Płatek, Nicolas Keller, Alexandre S. Dumon, Carine Michel, Philippe Sautet, Jacek Grams

Ru catalysts for levulinic acid hydrogenation with formic acid as a hydrogen source

Green Chem., 18, 2014–2028 (2016)

275) I. Gonzalez-Valls, A. Mirloup, T. Le Bahers, N. Keller, T. Cottineau, P. Sautet and V. Keller

Characterization and charge transfer properties of organic BODIPY dyes integrated in TiO₂ nanotube based dye-sensitized solar cells

RSC Adv. 6, 91529–91540 (2016)

276) Stephan N. Steinmann and Philippe Sautet

Assessing a First Principles Model of an Electrochemical Interface by Comparison with Experiment

J. Phys. Chem. C 120, 5619–5623 (2016)

277) Thuat T. Trinh, Xavier Rozanska, Françoise Delbecq, Alain Tuel and Philippe Sautet, Mechanism of Initial Step of Germanosilicate Formation in Solution:

a first-principles molecular dynamics study

PCCP, 18, 14419-14425 (2016)

278) Romain Réocreux, Minh Huynh, Carine Michel, Philippe Sautet
Controlling the Adsorption of Aromatic Compounds on Pt(111) with Oxygenate Substituents:
From DFT to Simple Molecular Descriptors
J. Phys. Chem. Lett. 7, 2074–2079 (2016)

279) Maxence Valla, Raphael Wischert, Aleix Comas-Vives, Matthew P. Conley, René Verel,
Christophe Copéret and Philippe Sautet
Role of Tricoordinate Al Sites in $\text{CH}_3\text{ReO}_3/\text{Al}_2\text{O}_3$ Olefin Metathesis Catalysts
J. Am. Chem. Soc. 138, 6774-6785 (2016)

280) Jérémie Zaffran, Carine Michel, Françoise Delbecq, Philippe Sautet
Towards more accurate prediction of activation energies for polyalcohol dehydrogenation on
transition metal catalysts in water
Catalysis Science & Technology, 6, 6615 – 6624 (2016)

281) Rodrigo Ferreira de Morais, Alejandro A. Franco, Philippe Sautet, David Loffreda
How Does the Surface Structure of Pt–Ni Alloys Control Water and Hydrogen Peroxide
Formation?
ACS Catal. 6, 5641–5650 (2016)

282) Ela Nurlaela, Hai Wang, Tatsuya Shinagawa, Sean Flanagan, Samy Ould-Chikh,
Muhammad Qureshi, Zoltán Mics, Philippe Sautet, Tangui Le Bahers, Enrique Cánovas,
Mischa Bonn, and Kazuhiro Takanabe
Enhanced Kinetics of Hole Transfer and Electrocatalysis during Photocatalytic Oxygen
Evolution by Cocatalyst Tuning
ACS Catal. 6, 4117–4126 (2016)

283) Evans A. Monyoncho, Stephan N. Steinmann, Carine Michel, Elena A. Baranova, Tom
K. Woo, Philippe Sautet
Ethanol Electro-oxidation on Palladium Revisited Using Polarization Modulation Infrared
Reflection Absorption Spectroscopy (PM-IRRAS) and Density Functional Theory (DFT):
Why Is It Difficult To Break the C–C Bond?
ACS Catal. 6, 4894–4906 (2016)

284) V. D'Anna, S. Norsic, D. Gajan, K. Sanders, A. J. Pell, A. Lesage, V. Monteil, C.
Copéret, G. Pintacuda, P. Sautet
Structural Characterization of the EtOH–TiCl₄–MgCl₂ Ziegler–Natta Precatalyst
J. Phys. Chem. C 120, 18075–18087 (2016)

285) R. Ferreira de Morais, T. Kerber, F. Calle-Vallejo, P. Sautet, D. Loffreda
Capturing Solvation Effects at a Liquid/Nanoparticle Interface by Ab Initio Molecular
Dynamics: Pt₂₀₁ Immersed in Water
Small 12, No. 38, 5312–5319 (2016)

286) S. N. Steinmann, C. Michel, R. Schwiedernoch, M. Wu, P. Sautet
Electro-carboxylation of butadiene and ethene over Pt and Ni catalysts
Journal of Catalysis 343 (2016) 240–247

- 287) S. T. A. G. Melissen, S. N. Steinmann, T. Le Bahers, P. Sautet
DFT Perspective on the Thermochemistry of Carbon Nitride Synthesis
J. Phys. Chem. C 2016, 120, 24542–24550
- 288) S. Petit, S.T.A.G. Melissen, L. Duclaux, M. T. Sougrati, T. Le Bahers, P. Sautet, D. Dambournet, O. Borkiewicz, C. Laberty-Robert, O. Durupthy
How Should Iron and Titanium be Combined in Oxides to Improve Photoelectrochemical Properties?
J. Phys. Chem. C 2016, 120, 24521–24532
- 289) E. Vignola, S. N. Steinmann, B.D. Vandegehuchte, D. Curulla, P. Sautet
C₂H₂-Induced Surface Restructuring of Pd–Ag Catalysts: Insights from Theoretical Modeling
J. Phys. Chem. C 2016, 120, 26320–26327
- 290) F. Göttl, C. Michel, P. C. Andrikopoulos, A.M. Love, J. Hafner, I. Hermans, P. Sautet
Computationally Exploring Confinement Effects in the Methane-to-Methanol Conversion Over Iron-Oxo Centers in Zeolites
ACS Catal. 2016, 6, 8404–8409
- 291) R. Réocreux, C.A. Ould Hamou, C. Michel, J. B. Giorgi, P. Sautet
Decomposition Mechanism of Anisole on Pt(111): Combining Single-Crystal Experiments and First-Principles Calculations
ACS Catal. 2016, 6, 8166–8178
- 292) F. Calle-Vallejo, M. D. Pohl, D. Reinisch, D. Loffreda, P. Sautet, A. S. Bandarenka
Why conclusions from platinum model surfaces do not necessarily lead to enhanced nanoparticle catalysts for the oxygen reduction reaction
Chem. Sci., 2017, DOI: 10.1039/C6SC04788B