Philippe Sautet - Publications in refereed international journals From 1987 to September 2025

1) P. Sautet, O. Eisenstein, K.M. Nicholas "Theoritical analysis of the addition of nucleophiles to (η4-diene) ML_n complexes".
Organometallics, 6, 1845-1849 (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, 2887-2894 (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 : Solid State Phys. 21, 3939-3957 (1988).

5) P. Sautet and C. Joachim "Electronic transmission coefficient for the single-impurity problem in the Scattering-matrix approach".
Physical Review B 38, 12238-12247 (1988).

6) P. Sautet and C. Joachim "Electronic interference produced by a benzene embedded in a polyacetylene chain".
Chemical Physics letters 153, 511-516 (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, 225-231 (1989).

8) P. Sautet and C. Joachim "The Sixl-Higelin salicylideneaniline molecular switch revisited".
Chemical Physics, 135, 99-108 (1989).

9) R.J. Cave, E.R. Davidson, P. Sautet, E. Canadell and O. Eisenstein "A theoretical Study of Models for X_2Y_2 Zintl Ions".
Journal of the American Chemical Society, 111, 8105-8111 (1989).

10) P. Sautet and C. Joachim "Calculation of the benzene on Rhodium STM images by the ESQC technique".
Chemical Physics Letters, 185, 23-30 (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, 245-260 (1991).

12) F. Delbecq and P. Sautet "η^1 versus η^2 coordination of aldehydes and ketones in organometallic complexes. A semi-empirical study".
Journal of the American Chemical Society, 114, 2446-2455 (1992).

13) P. Sautet and C. Joachim "Interpretation of large molecular adsorbate STM images: copper-phtalocyanine on copper"
Surface Science, 271, 387-394 (1992).

14) P. Sautet and C. Joachim "Are Electronic Interference Effects Important for STM Imaging of Substrates ans Adsorbates? A theoretical Analysis"
Ultramicroscopy, 42-44, 115-121 (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, 490-497 (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, 482-492 (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, 697-702 (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, 132-134 (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, 313-324 (1993)

21) F. Delbecq and P. Sautet "Low temperature adsorption of formaldehyde on a Pt(111) surface: A theoretical study"
Langmuir, 9, 197-207 (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, 7454-7461 (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, 2320-2328 (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, 400-410 (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$\sqrt{3}$x2$\sqrt{3}$)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 aldhydes 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 RuS_2 and its (100) and (111) surfaces"
Surface Science 336, 149-165 (1995)

41) J.C. Dunphy, P. Sautet, D.F. Ogletree and M. Salmeron "Approach to surface determination with the scanning tunneling microscope: Multipe-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, 63-72 (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, 4910-4925 (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, 8015-8027 (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-MoO_3 solid and study of the adsorption of H_2O 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 constrast 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 $Pt_{80}Fe_{20}$(111) alloy surface: a theoretical study of the adsorption of atomic H, CO and unsaturated molecules"
J. Catal., 164, 152-165 (1996)

50) H. Galloway, P. Sautet and M. Salmeron "Structure and contrast in Scanning Tunneling Microsocpy 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 MoS_2 surface"
Surface Science, 367, 209-220 (1996)

52) P. Sautet "Atomic adsorbate idenfication 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 "RuS_2 (111) surfaces: theoretical study of the various terminations and their interaction with H_2"
J. Catal., 170, 402-410 (1997)

57) F. Frechard and P. Sautet "Chemisorption of H_2 and H_2S on the (100) surface of RuS_2: 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 H_2 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, 15-23 (1998)

72) M.-L. Bocquet, P. Sautet
" Molecular transparence 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) F. Delbecq, P. Sautet
Interplay between magnetism and chemisorption: a theoretical study of CO and NO adsorption on a Pd3Mn alloy surface
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 microsocpy 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 Pd_3Mn 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 H_2 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 functionnal 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. Duclusaud, 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 MolecularDynamics 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
$Pt_{80}Fe_{20}$ 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, 23-29 (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, 71-86 (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, 2995-3002 (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, 115-126 (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, Anna Clotet, Josep M. Ricart, Françoise Delbecq, 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.MM 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, 11035-11043 (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, naphtalene, 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-Al_2O_3 surfaces on the stability and diffusion of single Pd atoms : A DFT Study"
J. Phys. Chem. B 110, 1759-1767 (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, 1339-1350 (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, 7392-7395 (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, 9157-9169 (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 H_2 and CH_4 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 C_2H_4 adsorption on $Pd_4/\gamma\text{-}Al_2O_3$**”**
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
“CH_3ReO_3 on $\gamma\text{-}Al_2O_3$: 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-Al_2O_3-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) Jérome 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) Jérome 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, 9274-9278 (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, 14693-14695 (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, 14456-14463 (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 CalculationsCombined 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 CalculationsCombined to Experiments. Part II: Hydroxylation Effects
J. Phys. Chem. C 112, 19710-19717 (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, TiO_2-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 Brönsted-Evans-Polanyi Relations: A Theoretical Insight
Angewandte Chemie International Edition, 48, 8978-8980 (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 aproach 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 Ni_3Pd 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 Vivrations 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 Pd_{13} and Pt_{13} / γ-Al_2O_3
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, 129-139 (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, 14928-14941 (2010)

197) David Coll, Françoise Delbecq, Yosslen Aray and Philippe Sautet
Stability of intermediates in the glycerol hydrogenolysison transition metal catalysts from first principles
PCCP **13**, 1448-1456 (2011)

198) E. Grinenval; 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, 18516-18528 (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, 19406-19414 (2010)

201) Christophe Mager-Maury, Gaëtan Bonnard, Céline Chizallet, Philippe Sautet and Pascal Raybaud

H_2 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, 2596-2603 (2011)

207) Rodrigo Ferreira de Morais, 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
Electrochemica 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 TiO_2 from first principles calculations"
J. Phys. Chem. C 115, 19394-19404 (2011)

213) Carine Michel, Florian Auneau, Françoise Delbecq, Philippe Sautet, "C-H versus O-H Bond Dissociation for Alcohols on a Rh(111) Surface: A Strong Assistance from Hydrogen Bonded Neighbors "
ACS catalysis, 1, 1430-1440 (2011)

214) X. Rozanska, P. Sautet, F. Delbecq, F. Lefebvre, S. Borshch, H. Chermette, J.M. Basset, E. Grinenval " 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 tetrapropylamonium 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, 474-479 (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-Al_2O_3: 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 Göltl, 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 $TiCl_4$/THF/$MgCl_2$: 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 $Al_2Cl_3Me_3$ 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 Göltl, 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. Takanabe, "Determination of the electronic structure and UV-Vis absorption properties of ($Na_{2-x}Cu_x$)Ta_4O_{11} from first-principle calculations"
J. Phys. Chem. C 117, 17277-17484 (2013)

233) Rosa E. Bulo, 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. Göltl, 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 Göltl 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. Göltl, 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, 2351-2358 (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, 3120-3124 (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 join experimental and theoretical study on levulinic acid conversion into gamma-valerolactone
Chem. Comm. 50, 12450-12453 (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. C 118, 15292-15299 (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 Ta_3N_5 particles
Chem. Mater. 26, 4812-4825 (2014)

248) Wenping Guo, Carine Michel, Renate Schwiedernoch, Raphael Wischert, Xin Xu, Philippe Sautet
Formation of acrylates from ethylene and CO_2 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, 20548-20560 (2014)

250) Hugo Petitjean, Hazar Guesmi, Hélène Lauron-Pernot, Guylène Costentin, David Loffreda, Philippe Sautet and Françoise Delbecq
How surface hydroxyls enhance MgO reactivity in basic catalysis: the case of MBOH conversion
ACS Catalysis, 4, 4004-4014 (2014)

251) Sigismund Teunis Alexander George Melissen, Frédéric Labat, Philippe Sautet, Tangui Le Bahers
Electronic properties of $PbX_3CH_3NH_3$ (X=Cl, Br, 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 ReOx 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 Auwarter, David Ecija, 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, 11392-11400 (2015)

258) A. M. Ruppert, J. Grams, M. Jedrzejczyk , J. Matras-Michalska, N. Keller, K. Ostojska, 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, 13949-13963 (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 Göltl, Philippe Sautet, and Ive Hermans
Can Dynamics Be Responsible for the Complex Multipeak 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 Göltl, 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 TiO_2 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 CH_3ReO_3/Al_2O_3 Olefin Metathesis Catalysts
J. Am. Chem. Soc. 138, 6774-6785 (2016)

280) Jérémie Zaffran, Carine Michel, Francoise 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: Pt_{201} 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
C_2H_2-Induced Surface Restructuring of Pd−Ag Catalysts: Insights from Theoretical Modeling
J. Phys. Chem. C 2016, 120, 26320−26327

290) F. Göltl, 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

291B) Stephan N. Steinmann, Philippe Sautet, Carine Michel
Solvation free energies for periodic surfaces: comparison of implicit and explicit solvation models
Phys. Chem. Chem. Phys., 2016, 18, 31850-31861

292) Stephan N. Steinmann, Sigismund T. A. G. Melissen, Tangui Le Bahers, Philippe Sautet
Challenges in calculating the bandgap of triazinebased carbon nitride structures
J. Mater. Chem. A, 2017, 5, 5115-5122

293) 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., 8, 2283-2289 (2017)

294) Pei Wang, Stephan N. Steinmann, Gang Fu, Carine Michel, Philippe Sautet
Key Role of Anionic Doping for H2 Production from Formic Acid on Pd(111)
ACS Catal. 2017, 7, 1955−1959

295) Ahmed Ziani, Claire Le Paven, Laurent Le Gendre, Florent Marlec, Ratiba Benzerga, Franck Tessier, François Cheviré, Mohamed N. Hedhili, Angel T. Garcia-Esparza, Sigismund Melissen, Philippe Sautet, Tangui Le Bahers, Kazuhiro Takanabe
Photophysical Properties of SrTaO2N Thin Films and Influence of Anion Ordering: A Joint Theoretical and Experimental Investigation

Chem. Mater. 2017, 29, 3989−3998

296) Cherif A. Ould Hamou, Romain Réocreux, Philippe Sautet, Carine Michel, Javier B. Giorgi
Adsorption and Decomposition of a Lignin β‑O‑4 Linkage Model, 2‑Phenoxyethanol, on Pt(111): Combination of Experiments and First-Principles Calculations
J. Phys. Chem. C 2017, 121, 9889−9900

297) A. Aloui, F. Delbecq, C. De Bellefon, P. Sautet
Understanding the influence of hydrogen pressure on the enantioselectivity of hydrogenation: A combined theory-experiment approach
Journal of Organometallic Chemistry 836-837 (2017) 90-99

298) Jean-David Rodier, Vincenza D'Anna, Nicolas Ritter, Serge Dalicieux, Philippe Sautet, Jean-Pierre Pascault, Alain Rousseau, Etienne Fleury
Isosorbide Telechelic Bio-Based Oligomers
JOURNAL OF POLYMER SCIENCE, PART A: POLYMER CHEMISTRY 2017, 55, 2178–2189

299) Anis Gannouni, Françoise Delbecq, Mongia Saïd Zina, Philippe Sautet
Oxidation of Methane to Methanol over Single Site Palladium Oxide Species on Silica: A Mechanistic view from DFT
J. Phys. Chem. A 2017, 121, 5500−5508

300) Emanuele Vignola, Stephan N. Steinmann, Bart D. Vandegehuchte, Daniel Curulla, Michail Stamatakis, Philippe Sautet
A machine learning approach to graph-theoretical cluster expansions of the energy of adsorbate layers
J. Chem. Phys. 147, 054106 (2017)

301) Florian Göltl, Philipp Müller, Pajean Uchupalanun, Philippe Sautet, Ive Hermans
Developing a Descriptor-Based Approach for CO and NO Adsorption Strength to Transition Metal Sites in Zeolites
Chem. Mater. 2017, 29, 6434−6444

302) Stephan N. Steinmann, Paul Fleurat-Lessard, Andreas W. Götz, Carine Michel, Rodrigo Ferreira de Morais, Philippe Sautet
Molecular Mechanics Models for the Image Charge, a Comment on "Including Image Charge Effects in the Molecular Dynamics Simulations of Molecules on Metal Surfaces"
Journal of Computational Chemistry 2017, 38, 2127–2129

303) Geun Ho Gu, Benjamin Schweitzer, Carine Michel, Stephan N. Steinmann, Philippe Sautet, Dionisios G. Vlachos
Group Additivity for Aqueous Phase Thermochemical Properties of Alcohols on Pt(111)
J. Phys. Chem. C 2017, 121, 21510−21519

304) Amal BaQais, Antton Curutchet, Ahmed Ziani, Hassan Ait Ahsaine, Philippe Sautet, Kazuhiro Takanabe, Tangui Le Bahers
Bismuth Silver Oxysulfide for Photoconversion Applications: Structural and Optoelectronic Properties

Chem. Mater. 2017, 29, 8679−8689

305) Sarah Gautier, Philippe Sautet
Coadsorption of Butadiene and Hydrogen on the (111) Surfaces of Pt and Pt_2Sn Surface Alloy: Understanding the Cohabitation from First-Principles Calculations
J. Phys. Chem. C 2017, 121, 25152-25163

306) Tao Wang, Zhen Yan, Carine Michel, Marc Pera-Titus, Philippe Sautet
Trends and Control in the Nitridation of Transition Metal Surfaces
ACS Catal. 2018, 8, 63−68

307) Alexandre S. Dumon, Tao Wang, Javier Ibañez, Ajay Tomer, Zhen Yan, Raphael Wischert, Philippe Sautet, Marc Pera-Titus, Carine Michel
Direct n-octanol amination by ammonia on supported Ni and Pd catalysts: activity is enhanced by “spectator” ammonia adsorbates
Catal. Sci. Technol., 2018, 8, 611-621

308) Sun, G.; Sautet, P.,
Metastable Structures in Cluster Catalysis from First-Principles: Structural Ensemble in Reaction Conditions and Metastability Triggered Reactivity
J. Am. Chem. Soc. 2018, 140, 2812−2820

309) Emanuele Vignola, Stephan N. Steinmann, Ahmad Al Farra, Bart D. Vandegehuchte, Daniel Curulla, Philippe Sautet
Evaluating the Risk of C−C Bond Formation during Selective Hydrogenation of Acetylene on Palladium
ACS Catal. 2018, 8, 1662−1671

310) John C. Thomas, Dominic P. Goronzy, Andrew C. Serino, Harsharn S. Auluck, Olivia R. Irving, Elisa Jimenez-Izal, Jacqueline M. Deirmenjian, Jan Macháček, Philippe Sautet, Anastassia N. Alexandrova, Tomáš Baše, Paul S. Weiss
Acid−Base Control of Valency within Carboranedithiol Self-Assembled Monolayers: Molecules Do the Can-Can
ACS Nano 2018, 12, 2211−2221

311) Evans A. Monyoncho, Stephan N. Steinmann, Philippe Sautet, Elena A. Baranova, Carine Michel
Computational screening for selective catalysts: Cleaving the C-C bond during ethanol electro-oxidation reaction
Electrochimica Acta 274 (2018) 274-278

312) Stephan N. Steinmann, Rodrigo Ferreira De Morais, Andreas W. Götz, Paul Fleurat-Lessard, Marcella Iannuzzi, Philippe Sautet, Carine Michel
Force Field for Water over Pt(111): Development, Assessment, and Comparison
J. Chem. Theory Comput. 2018, 14, 3238−3251

313) Xiaobo Li, Sigismund T. A. G. Melissen, Tangui Le Bahers, Philippe Sautet, Anthony F. Masters, Stephan N. Steinmann, Thomas Maschmeyer
Shining Light on Carbon Nitrides: Leveraging Temperature To Understand Optical Gap Variations

Chem. Mater. 2018, 30, 4253−4262

314) Emanuele Vignola, Stephan N. Steinmann, Katell Le Mapihan, Bart D. Vandegehuchte, Daniel Curulla, Philippe Sautet
Acetylene Adsorption on Pd−Ag Alloys: Evidence for Limited Island Formation and Strong Reverse Segregation from Monte Carlo Simulations
J. Phys. Chem. C 2018, 122, 15456−15463

315) Muhammad Qureshi, Angel T. Garcia-Esparza, Tatsuya Shinagawa, Philippe Sautet, Tangui Le Bahers, Kazuhiro Takanabe
Contribution of electrolyte in nanoscale electrolysis of pure and buffered water by particulate photocatalysis
Sustainable Energy Fuels, 2018, 2, 2044-2052

316) Agnieszka M. Ruppert, Marcin Jędrzejczyk, Natalia Potrzebowska, Kamila Kaźmierczak, Magdalena Brzezińska, Olga Sneka-Płatek, Philippe Sautet, Nicolas Keller, Carine Michel, Jacek Grams
Supported gold–nickel nano-alloy as a highly efficient catalyst in levulinic acid hydrogenation with formic acid as an internal hydrogen source
Catal. Sci. Technol., 2018, 8, 4318-4331

317) Ka Wing Chan, Erwin Lam, Vincenza D'Anna, Florian Allouche, Carine Michel, Olga V. Safonova, Philippe Sautet, Christophe Copéret
C−H Activation and Proton Transfer Initiate Alkene Metathesis Activity of the Tungsten(IV)−Oxo Complex
J. Am. Chem. Soc. 2018, 140, 11395−11401

318) Pierre-Adrien Payard, Qingyi Gu, Wenping Guo, Qianran Wang, Matthieu Corbet, Carine Michel, Philippe Sautet, Laurence Grimaud, Raphael Wischert, Marc Pera-Titus
Direct Amination of Alcohols Catalyzed by Aluminum Triflate: An Experimental and Computational Study
Chem. Eur. J. 2018, 24, 14146 – 14153

319) Anis Gannouni, Carine Michel, Françoise Delbecq, Mongia Saïd Zinaa, Philippe Sautet
DFT investigations for the catalytic reaction mechanism of methane combustion occurring on Pd(II)/Al-MCM-41
Phys.Chem.Chem.Phys., 2018, 20, 25377-25386

320) Qingyi Gu, Philippe Sautet, Carine Michel
Unraveling the Role of Base and Catalyst Polarization in Alcohol Oxidation on Au and Pt in Water
ACS Catal. 2018, 8, 11716−11721

321) Wei Zhao, Céline Chizallet, Philippe Sautet, Pascal Raybaud
Dehydrogenation mechanisms of methyl-cyclohexane on γ-Al2O3 supported Pt_{13}: Impact of cluster ductility
Journal of Catalysis 370 (2019) 118–129

322) Matthijs A. van Spronsen, Kaining Duanmu, Christopher R. O'Connor, Tobias Egle, Heath Kersell, Judit Oliver-Meseguer, Miquel B. Salmeron, Robert J. Madix, Philippe Sautet, Cynthia M. Friend
Dynamics of Surface Alloys: Rearrangement of Pd/Ag(111) Induced by CO and O_2
J. Phys. Chem. C 2019, 123, 8312−8323

323) Jérôme Joubert, Françoise Delbecq, and Philippe Sautet
Unravelling the Metastable Nature of the Single Site Tungsten Hydride Metathesis Catalyst Supported on γ‑Alumina from First Principles
J. Phys. Chem. C 2019, 123, 1226–1234

324) Federico Calle-Vallejo, Rodrigo F. de Morais, Francesc Illas, David Loffreda, Philippe Sautet
Affordable Estimation of Solvation Contributions to the Adsorption Energies of Oxygenates on Metal Nanoparticles
J. Phys. Chem. C 2019, 123, 5578−5582

325) Addis S. Fuhr, Philippe Sautet, and Anastassia N. Alexandrova
Heterogeneity in Local Chemical Bonding Explains Spectral Broadening in Quantum Dots with Cu Impurities
J. Phys. Chem. C 2019, 123, 5705−5713

326) George Yan, Tobias Wähler, Ralf Schuster, Matthias Schwarz, Chantal Hohner, Kristin Werner, Jörg Libuda, Philippe Sautet
Water on Oxide Surfaces: A Triaqua Surface Coordination Complex on Co3O4(111)
J. Am. Chem. Soc. 2019, 141, 5623−5627

327) Stephan N. Steinmann, Zi-Yang Wei, Philippe Sautet
Theory and experiments join force to characterize the electrocatalytic interface
Proc. Natl. Acad. Sci. USA, 2019, 116, 7611-7613. DOI : 10.1073/pnas.1903412116

328) Mufan Li, Kaining Duanmu, Chengzhang Wan, Tao Cheng, Liang Zhang, Sheng Dai, Wenxin Chen, Zipeng Zhao, Peng Li, Huilong Fei, Yuanming Zhu, Rong Yu, Jun Luo, Ketao Zang, Zhaoyang Lin, Mengning Ding, Jin Huang, Hongtao Sun, Xiaoqing Pan, Jinghua Guo, William A. Goddard III, Philippe Sautet, Yu Huang, Xiangfeng Duan, Single-atom tailoring of platinum nanocatalysts for high-performance multifunctional electrocatalysis, Nature Catalysis, **2**, 495–503 (2019)

329) Romain Réocreux, Etienne Girel, Paul Clabaut, Alain Tuel, Michèle Besson, Alexandra Chaumonnot, Amandine Cabiac, Philippe Sautet, and Carine Michel
Reactivity of shape-controlled crystals and metadynamics simulations locate the weak spots of alumina in water
Nature communications 2019, 10, 3139

330) George Yan, Philippe Sautet
Surface Structure of Co_3O_4(111) under Reactive Gas-Phase Environments
ACS Catal. 2019, 9, 6380−6392

331) Rik V. Mom, Sigismund T. A. G. Melissen, Philippe Sautet, Joost W. M. Frenken, Stephan N. Steinmann, Irene M. N. Groot

The Pressure Gap for Thiols: Methanethiol Self-Assembly on Au(111) from Vacuum to 1 bar
J. Phys. Chem. C 2019, 123, 12382−12389

332) Bin Zhang, Geng Sun, Shipeng Ding, Hiroyuki Asakura, Jia Zhang, Philippe Sautet, Ning Yan
Atomically Dispersed Pt1−Polyoxometalate Catalysts: How Does Metal−Support Interaction Affect Stability and Hydrogenation Activity?
J. Am. Chem. Soc. 2019, 141, 8185−8197

333) Jin Soo Lim, Nicola Molinari, Kaining Duanmu, Philippe Sautet, Boris Kozinsky
Automated Detection and Characterization of Surface Restructuring Events in Bimetallic Catalysts
J. Phys. Chem. C, 2019, 123, 26, 16332-16344

334) Tao Wang, Javier Ibañez, Kang Wang, Lin Fang, Maarten Sabbe, Carine Michel, Sébastien Paul, Marc Pera-Titus, Philippe Sautet
Rational design of selective metal catalysts for alcohol amination with ammonia
Nature Catalysis, 2019, 2, 773–779

335) Romain Réocreux, Tao Jiang, Marcella Iannuzzi, Carine Michel, Philippe Sautet
Structuration and Dynamics of Interfacial Liquid Water at Hydrated γ‑Alumina Determined by ab Initio Molecular Simulations: Implications for Nanoparticle Stability
ACS Appl. Nano Mater. 2018, 1, 191−199

336) Geng Sun, Philippe Sautet, Toward Fast and Reliable Potential Energy Surfaces for Metallic Pt Clusters by Hierarchical Delta Neural Networks, J. Chem. Theory Comput. 2019, 15, 5614-5627.

337) Yan Tang, Chithra Asokan, Mingjie Xu, George W. Graham, Xiaoqing Pan, Phillip Christopher, Jun Li, Philippe Sautet, Rh single atoms on TiO_2 dynamically respond to reaction conditions by adapting their site, Nature communications 2019, 10, 4488

338) George Yan and Philippe Sautet, Correction to “The Surface Structure of Co_3O_4(111) under Reactive Gas-Phase Environments”
ACS Catal. 2019, 9, 8980−8984

339) Sara A. Azzam, Faisal H. Alshafei, Tirso López-Ausens, Richa Ghosh, Akash N. Biswas, Philippe Sautet, Sergey Prikhodko, and Dante A. Simonetti, Effects of Morphology and Surface Properties of Copper Oxide on the Removal of Hydrogen Sulfide from Gaseous Streams
Ind. Eng. Chem. Res. 2019, 58, 18836−18847

340) Geng Sun, Anastassia N. Alexandrova, and Philippe Sautet, Pt_8 cluster on alumina under a pressure of hydrogen: Support-dependent reconstruction from first-principles global optimization
J. Chem. Phys. 2019, 151, 194703

341) Romain Réocreux, Carine Michel, Paul Fleurat-Lessard, Philippe Sautet, Stephan N. Steinmann, Evaluating Thermal Corrections for Adsorption Processes at the Metal/Gas Interface,

J. Phys. Chem. C 2019, 123, 28828−28835

342) Huanchen Zhai, Philippe Sautet and Anastassia N. Alexandrova, Global Optimization of Adsorbate Covered Supported Cluster Catalysts: The Case of $Pt_7H_{10}CH_3$ on α-Al_2O_3
ChemCatChem 2019, 12, 762-770

343) Qingyi Gu, Philippe Sautet, and Carine Michel, Correction to "Unraveling the Role of Base and Catalyst Polarization in Alcohol Oxidation on Au and Pt in Water"
ACS Catal. 2019, 9, 6541−6542

344) Mathilde Luneau, Tanya Shirman, Alexandre C. Foucher, Kaining Duanmu, David M.A. Verbart, Philippe Sautet, Eric A. Stach, Joanna Aizenberg, Robert J. Madix, Cynthia M. Friend, Achieving High Selectivity for Alkyne Hydrogenation at High Conversions with Compositionally Optimized PdAu Nanoparticle Catalysts in Raspberry Colloid-Templated SiO_2
ACS Catal. 2020, 10, 441−450

345) Rui Shang, Stephan N. Steinmann, Bo-Qing Xu, Philippe Sautet, Mononuclear Fe in N-doped carbon: computational elucidation of active sites for electrochemical oxygen reduction and oxygen evolution reactions,
Catal. Sci. Technol., 2020, 10, 1006–1014

346) Wei Chen, Lixin Sun, Boris Kozinsky, Cynthia M. Friend, Efthimios Kaxiras, Philippe Sautet, Robert J. Madix, Effect of Frustrated Rotations on the Pre-Exponential Factor for Unimolecular Reactions on Surfaces: A Case Study of Alkoxy Dehydrogenation,
J. Phys. Chem. C 2020, 124, 1429−1437

347) Geng Sun, Anastassia N. Alexandrova, Philippe Sautet, Structural Rearrangements of Subnanometer Cu Oxide Clusters Govern Catalytic Oxidation,
ACS Catal. 2020, 10, 5309−5317

348) Han Guo, Philippe Sautet, Anastassia N. Alexandrova, Reagent-Triggered Isomerization of Fluxional Cluster Catalyst via Dynamic Coupling
J. Phys. Chem. Lett. 2020, 11, 3089-3094

349) Heath Kersell, Zahra Hooshmand, George Yan, Duy Le, Huy Nguyen, Baran Eren, Cheng Hao Wu, Iradwikanari Waluyo, Adrian Hunt, Slavomír Nemšák, Gabor Somorjai, Talat S. Rahman, Philippe Sautet, Miquel Salmeron, CO Oxidation Mechanisms on CoO_x-Pt Thin Films
J. Am. Chem. Soc. 2020, 142, 8312−8322

350) Mustafa Karatok, Kaining Duanmu, Christopher R. O'Connor, Jorge Anibal Boscoboinik, Philippe Sautet, Robert J. Madix, Cynthia M. Friend, Tuning reactivity layer-by-layer: formic acid activation on Ag/Pd(111)
Chem. Sci., 2020, 11, 6492–6499

351) Constantin A. Walenta, Fang Xu, Celine Tesvara, Christopher R. O'Connor, Philippe Sautet, Cynthia M. Friend, Facile Decomposition of Organophosphonates by Dual Lewis Sites on a Fe_3O_4(111) Film
J. Phys. Chem. C 2020, 124, 12432−12441

352) Addis S. Fuhr, Anastassia N. Alexandrova, Philippe Sautet, Stoichiometry-controllable optical defects in $Cu_xIn_{2-x}S_y$ quantum dots for energy harvesting
J. Mater. Chem. A, 2020, 8, 12556–12565

353) Xia Sang, Yantao Xia, Philippe Sautet, Jane P. Chang, Atomic layer etching of metals with anisotropy, specificity, and selectivity
J. Vac. Sci. Technol. A 38, 043005 (2020)

354) Lele Peng, Ziyang Wei, Chengzhang Wan, Jing Li, Zhuo Chen, Dan Zhu, Daniel Baumann, Haotian Liu, Christopher S. Allen, Xiang Xu, Angus I. Kirkland, Imran Shakir, Zeyad Almutairi, Sarah Tolbert, Bruce Dunn, Yu Huang, Philippe Sautet, Xiangfeng Duan, A fundamental look at electrocatalytic sulfur reduction reaction, *Nat Catal* **3,** 762–770 (2020). https://doi.org/10.1038/s41929-020-0498-x

355) Jin Soo Lim, Jonathan Vandermause, Matthijs A. van Spronsen, Albert Musaelian, Yu Xie, Lixin Sun, Christopher R. O'Connor, Tobias Egle, Nicola Molinari, Jacob Florian, Kaining Duanmu, Robert J. Madix, Philippe Sautet, Cynthia M. Friend, and Boris Kozinsky, Evolution of Metastable Structures at Bimetallic Surfaces from Microscopy and Machine-Learning Molecular Dynamics
J. Am. Chem. Soc. 2020, 142, 15907−15916, DOI: 10.1021/jacs.0c06401

356) Olga Sneka-Płatek, Kamila Kaźmierczak, Marcin Jędrzejczyk, Philippe Sautet, Nicolas Keller, Carine Michel, Agnieszka M. Ruppert, Understanding the influence of the composition of the Ag-Pd catalysts on the selective formic acid decomposition and subsequent levulinic acid hydrogenation,
International Journal of Hydrogen Energy, 45, 2020, 17339-17353

357) Borna Zandkarimi, Geng Sun, Avik Halder, Soenke Seifert, Stefan Vajda, Philippe Sautet, and Anastassia N. Alexandrova, Interpreting the Operando XANES of Surface-Supported Subnanometer Clusters: When Fluxionality, Oxidation State, and Size Effect Fight The Journal of Physical Chemistry C 2020 124, 10057-10066

358) Vaidish Sumaria, Luan Nguyen, Franklin Feng Tao, and Philippe Sautet, Optimal Packing of CO at a High Coverage on Pt(100) and Pt(111) Surfaces
ACS Catalysis 2020, 10, 9533-9544

359) Christopher R. O'Connor, Kaining Duanmu, Dipna A. Patel, Eri Muramoto, Matthijs A. van Spronsen, Dario Stacchiola, E. Charles H. Sykes, Philippe Sautet, Robert J. Madix, Cynthia M. Friend, Facilitating hydrogen atom migration via a dense phase on palladium islands to a surrounding silver surface, Proceedings of the National Academy of Sciences 2020, 117, 22657-22664; DOI: 10.1073/pnas.2010413117

360) Qizhang Yan, Grace Whang, Ziyang Wei, Shu-Ting Ko, Philippe Sautet, Sarah H. Tolbert, Bruce S. Dunn, Jian Luo, A Perspective on Interfacial Engineering of Lithium Metal Anodes and Beyond, Appl. Phys. Lett. **117**, 080504 (2020)

361) Sara A. Azzam, Alexey Boubnov, Adam S. Hoffman, Tirso López-Ausens, Nicole Chiang, Griffin Canning, Philippe Sautet, Simon R. Bare, Dante A. Simonetti, Insights into

Copper Sulfide Formation from Cu and S K-edge XAS and DFT studies, Inorg. Chem. 2020, 59, 20, 15276–15288

362) Fang Liu, Geng Sun, Hao Bin Wu, Gen Chen, Duo Xu, Ruiwei Mo, Li Shen, Xianyang Li, Shengxiang Ma, Ran Tao, Xinru Li, Xinyi Tan, Bin Xu, Ge Wang, Bruce S. Dunn, Philippe Sautet, Yunfeng Lu, Dual redox mediators accelerate the electrochemical kinetics of lithium-sulfur batteries. Nat Commun 11, 5215 (2020).

363) Mathilde Luneau, Jin Soo Lim, Dipna A. Patel, E. Charles H. Sykes, Cynthia M. Friend, Philippe Sautet, Guidelines to achieving high selectivity for the hydrogenation of α–β unsaturated aldehydes with bimetallic and dilute alloy catalysts − A review, Chem. Rev. 2020, 120, 23, 12834–12872

364) Tieqiang Zeng, Geng Sun, Changxi Miao, George Yan, Yingchun Ye, Weimin Yang, Philippe Sautet, Stabilizing Oxidative Dehydrogenation Active Site at High Temperature with Steam: $ZnFe_2O_4$ Catalyzed Oxidative Dehydrogenation of 1-Butene to 1,3-Butadiene, *ACS Catal.* 2020, 10, 21, 12888–12897

365) Zisheng Zhang, Zhi-Hao Cui, Elisa Jimenez-Izal, Philippe Sautet, and Anastassia N. Alexandrova, Hydrogen Evolution on Restructured B‑Rich WB: Metastable Surface States and Isolated Active Sites, ACS Catal. 2020, 10, 13867−13877

366) Sigismund T. A. G. Melissen, Tangui Le Bahers, Philippe Sautet, Stephan N. Steinmann, What does graphitic carbon nitride really look like? Physical Chemistry Chemical Physics, 2021, 23, 2853 – 2859

367) Geng Sun, Jack T. Fuller, Anastassia N. Alexandrova, and Philippe Sautet, Global Activity Search Uncovers Reaction Induced Concomitant Catalyst Restructuring for Alkane Dissociation on Model Pt Catalysts, ACS Catalysis 2021 11, 1877-1885 . DOI: 10.1021/acscatal.0c05421

368) Max J. Hülsey, Geng Sun, Philippe Sautet, and Ning Yan, Observing Single-Atom Catalytic Sites During Reactions with Electrospray Ionization Mass Spectrometry, Angew. Chem. Int. Ed. 2021, 60, 4764–4773

369) Jessi E. S. van der Hoeven, Hio Tong Ngan, Austin Taylor, Nathaniel M. Eagan, Joanna Aizenberg, Philippe Sautet, Robert J. Madix, and Cynthia M. Friend, Entropic Control of HD Exchange Rates over Dilute Pd-in-Au Alloy Nanoparticle Catalysts, ACS Catal. 2021, 11, 6971−6981

370) Marine Ciantar, Thuat T. Trinh, Carine Michel, Philippe Sautet, Caroline Mellot-Draznieks, Carlos Nieto-Draghi, Impact of Organic Templates on the Selective Formation of Zeolite Oligomers, Angew. Chem. Int. Ed. 2021, 60, 7111–7116

371) Grace Whang, Qizhang Yan, Da Li, Ziyang Wei, Danielle Butts, Philippe Sautet, Jian Luo, Bruce Dunn, Avoiding dendrite formation by confining lithium deposition underneath Li–Sn coatings, Journal of materials research, 36, 797–811, 2021.

372) Ziyang Wei, Shona M. Becwar, Bradley F. Chmelka, and Philippe Sautet, Atomic Environments in N‑Containing Graphitic Carbon Probed by First-Principles Calculations and

Solid-State Nuclear Magnetic Resonance, J. Phys. Chem. C 2021, 125, 8779−8787

373) Junjie Shi, Cameron J. Owen, Hio Tong Ngan, Siyu Qin, Vikram Mehar, Philippe Sautet, Jason F. Weaver, Formation of a Ti–Cu(111) single atom alloy: Structure and CO binding, J. Chem. Phys. 154, 234703 (2021)

374) Simran Kumari and Philippe Sautet, Highly dispersed Pt atoms and clusters on hydroxylated indium tin oxide: a view from first-principles calculations, J. Mater. Chem. A, 2021, 9, 15724-15733

375) Yantao Xia and Philippe Sautet, Thermodynamics of Atomic Layer Etching Chemistry on Copper and Nickel Surfaces from First Principles, Chem. Mater. 2021, 33, 6774-6786

376) Tao Wang, Jin Sha, Maarten Sabbe, Philippe Sautet, Marc Pera-Titus, Carine Michel, Identification of active catalysts for the acceptorless dehydrogenation of alcohols to carbonyls. *Nat Commun* **12,** 5100 (2021).

377) Manuel J. Kolb, David Loffreda, Philippe Sautet, Federico Calle-Vallejo, Structure-sensitive scaling relations among carbon-containing species and their possible impact on CO_2 electroreduction, Journal of Catalysis 395, 136–142 (2021)

378) Geng Sun and Philippe Sautet, Active Site Fluxional Restructuring as a New Paradigm in Triggering Reaction Activity for Nanocluster Catalysis, Acc. Chem. Res., 2021, 54, 3841-3849

379) Alexis Sangnier, Eric Genty, Mathilde Iachella, Philippe Sautet, Pascal Raybaud, Mickaël Matrat, Christophe Dujardin, Céline Chizallet, Thermokinetic and Spectroscopic Mapping of Carbon Monoxide Adsorption on Highly Dispersed Pt/γ-Al_2O_3, *ACS Catal.* **2021** *11*, 13280-13293

380) Vaidish Sumaria, Philippe Sautet, CO organization at ambient pressure on stepped Pt surfaces: first principles modeling accelerated by neural networks, Chemical Science, 2021, 12, 15543 - 15555.

381) Ziyang Wei, Florian Göltl, Philippe Sautet, Diffusion Barriers for Carbon Monoxide on the Cu(001) Surface Using Many-Body Perturbation Theory and Various Density Functionals, Journal of Chemical Theory and Computation, **2021** *17*, 7862-7872

382) Georgios Giannakakis, Paul Kress, Kaining Duanmu, Hio Tong Ngan, George Yan, Adam S. Hoffman, Zhen Qi, Antonios Trimpalis, Leelavathi Annamalai, Mengyao Ouyang, Jilei Liu, Nathaniel Eagan, Juergen Biener, Dimosthenis Sokaras, Maria Flytzani-Stephanopoulos, Simon R. Bare, Philippe Sautet, and E. Charles H. Sykes, Mechanistic and Electronic Insights into a Working NiAu Single-Atom Alloy Ethanol Dehydrogenation Catalyst, Journal of the American Chemical Society 2021, 143, 21567-21579

383) Eri Muramoto, Wei Chen, Xiwen Jia, Cynthia M. Friend, Philippe Sautet, Robert J. Madix, Toward benchmarking theoretical computations of elementary rate constants on catalytic surfaces: formate decomposition on Au and Cu, *Chem. Sci.*, 2022, 13, 804-815

384) Han Guo, Patricia Poths, Philippe Sautet, and Anastassia N. Alexandrova, Oxidation Dynamics of Supported Catalytic Cu Clusters: Coupling to Fluxionality, *ACS Catalysis* **2022** *12* (1), 818-827

385) Ziyang Wei, Philippe Sautet, Revisiting the link between magnetic properties and chemisorption at graphene nanoribbon zigzag edge, J. Chem. Phys. 156, 044706 (2022)

386) Yan, G.; Tang, Y.; Li, Y.; Nguyen, L.; Sakata, T; Higashi, K.; Tao, F.; Sautet, P. Reaction product-driven restructuring and assisted stabilization of a highly dispersed Rh-on-ceria catalyst. *Nat Catal* **5,** 119–127 (2022).

387) Patricia Poths, Geng Sun, Philippe Sautet, and Anastassia N. Alexandrova, Interpreting the Operando X-ray Absorption Near-Edge Structure of Supported Cu and CuPd Clusters in Conditions of Oxidative Dehydrogenation of Propane: Dynamic Changes in Composition and Size, *The Journal of Physical Chemistry C* **2022** *126* (4), 1972-1981

388) Nicholas Marcella, Jin Soo Lim, Anna M. Plonka, George Yan, Cameron J. Owen, Jessi E. S. van der Hoeven, Alexandre C. Foucher, Hio Tong Ngan, Steven B. Torrisi, Nebojsa S. Marinkovic, Eric A. Stach, Jason F. Weaver, Joanna Aizenberg, Philippe Sautet, Boris Kozinsky, Anatoly I. Frenkel, Decoding reactive structures in dilute alloy catalysts. *Nat Commun* **13,** 832 (2022)

389) Jennifer D. Lee, Jeffrey B. Miller, Anna V. Shneidman, Lixin Sun, Jason F. Weaver, Joanna Aizenberg, Juergen Biener, J. Anibal Boscoboinik, Alexandre C. Foucher, Anatoly I. Frenkel, Jessi E. S. van der Hoeven, Boris Kozinsky, Nicholas Marcella, Matthew M. Montemore, Hio Tong Ngan, Christopher R. O'Connor, Cameron J. Owen, Dario J. Stacchiola, Eric A. Stach, Robert J. Madix, Philippe Sautet and Cynthia M. Friend, Dilute Alloys Based on Au, Ag, or Cu for Efficient Catalysis: From Synthesis to Active Sites. *Chemical Reviews* **2022** *122*, 8758-8808

390) Ziyang Wei, Florian Göltl, Stephan N. Steinmann and Philippe Sautet, Modeling Electrochemical Processes with Grand Canonical Treatment of Many-Body Perturbation Theory, J. Phys. Chem. Lett. 2022, 13, 6079−6084

391) Chen Zhou, Hio Tong Ngan, Jin Soo Lim, Zubin Darbari, Adrian Lewandowski, Dario J. Stacchiola, Boris Kozinsky, Philippe Sautet and Jorge Anibal Boscoboinik, Dynamical Study of Adsorbate-Induced Restructuring Kinetics in Bimetallic Catalysts Using the PdAu(111) Model System, J. Am. Chem. Soc. 2022, 144, 15132−15142

392) Ziyang Wei and Philippe Sautet, Improving the Accuracy of Modelling CO_2 Electroreduction on Copper Using Many-Body Perturbation Theory, Angew. Chem.Int. Ed. 2022, e202210060

393) Jennifer D. Lee, Zhen Qi, Alexandre C. Foucher, Hio Tong Ngan, Kevin Dennis, Jun Cui, Ilia I. Sadykov, Ethan J. Crumlin, Philippe Sautet, Eric A. Stach, Cynthia M. Friend, Robert J. Madix, and Juergen Biener, Facilitating Hydrogen Dissociation over Dilute Nanoporous Ti−Cu Catalysts, J. Am. Chem. Soc. 2022, 144, 16778−16791

394) Celine Tesvara, Constantin Walenta and Philippe Sautet, Oxidative decomposition of dimethyl methylphosphonate on rutile TiO_2(110): the role of oxygen vacancies, Phys. Chem. Chem. Phys., 2022, 24, 23402

395) Jessi E. S. van der Hoeven, Hio Tong Ngan, George Yan, Joanna Aizenberg, Robert J. Madix, Philippe Sautet, and Cynthia M. Friend, Unraveling 1‑Hexene Hydrogenation over Dilute Pd-in-Au Alloys, *The Journal of Physical Chemistry C* **2022** *126*, 15710-15723

396) Eri Muramoto, Dipna A. Patel, Wei Chen, Philippe Sautet, E. Charles H. Sykes, and Robert J. Madix, Direct Observation of Solvent−Reaction Intermediate Interactions in Heterogeneously Catalyzed Alcohol Coupling, *Journal of the American Chemical Society* **2022** *144*, 17387-17398

397) Hio Tong Ngan, George Yan, Jessi E. S. van der Hoeven, Robert J. Madix, Cynthia M. Friend, Philippe Sautet, Hydrogen dissociation controls 1-hexyne selective hydrogenation on dilute Pd-in-Au catalysts, ACS Catal. 2022, 12, 13321−13333

398) Zisheng Zhang, Ziyang Wei, Philippe Sautet, Anastassia N. Alexandrova, Hydrogen-Induced Restructuring of a Cu(100) Electrode in Electroreduction Conditions, J. Am. Chem. Soc. 2022, 144, 42, 19284–19293

399) Julen Munarriz, Zisheng Zhang, Philippe Sautet, and Anastassia N. Alexandrova, Graphite-Supported Pt_n Cluster Electrocatalysts: Major Change of Active Sites as a Function of the Applied Potential, ACS Catal. 2022, 12, 23, 14517–14526

400) Hua An, Geng Sun, Max J. Hülsey, Philippe Sautet, and Ning Yan, Demonstrating the Electron−Proton-Transfer Mechanism of Aqueous Phase 4‑Nitrophenol Hydrogenation Using Unbiased Electrochemical Cells, ACS Catal. 2022, 12, 15021–15027

401) Yantao Xia, Philippe Sautet, Plasma Oxidation of Copper: Molecular Dynamics Study with Neural Network Potentials, *ACS Nano* 2022, 16, 20680–20692

402) Vaidish Sumaria, Luan Nguyen, Franklin Feng Tao, Philippe Sautet, Atomic-Scale Mechanism of Platinum Catalyst Restructuring under a Pressure of Reactant Gas, *J. Am. Chem. Soc.* 2023, 145, 1, 392–401

403) Mustafa Karatok, Hio Tong Ngan, Xiwen Jia, Christopher R. O'Connor, J. Anibal Boscoboinik, Dario J. Stacchiola, Philippe Sautet, Robert J. Madix, Achieving Ultra-High Selectivity to Hydrogen Production from Formic Acid on Pd–Ag Alloys, *J. Am. Chem. Soc.* 2023, 145, 5114–5124

404) Simran Kumari, Tsugunosuke Masubuchi, Henry S. White, Anastassia Alexandrova, Scott L. Anderson, Philippe Sautet, Electrocatalytic Hydrogen Evolution at Full Atomic Utilization over ITO-Supported Sub-nano-Pt_n Clusters: High, Size-Dependent Activity Controlled by Fluxional Pt Hydride Species, *J. Am. Chem. Soc.* 2023, 145, 5834-5845 https://doi.org/10.1021/jacs.2c13063

405) Simran Kumari and Philippe Sautet, Elucidation of the Active Site for the Oxygen Evolution Reaction on a Single Pt Atom Supported on Indium Tin Oxide, J. Phys. Chem. Lett. 14, 2635−2643 (2023)

406) Dipna A. Patel, Georgios Giannakakis, George Yan, Hio Tong Ngan, Peng Yu, Ryan T. Hannagan, Paul L. Kress, Junjun Shan, Prashant Deshlahra, Philippe Sautet, E. Charles H. Sykes, Mechanistic Insights into Nonoxidative Ethanol Dehydrogenation on NiCu Single-Atom Alloys, *ACS Catal.* 2023, 13, 4290–4303

407) Kangze Shen, Simran Kumari, Yu-Chao Huang, Joonbaek Jang, Philippe Sautet, and Carlos G. Morales-Guio, Electrochemical Oxidation of Methane to Methanol on Electrodeposited Transition Metal Oxides
Journal of the American Chemical Society, 2023, 145, 6927-6943

408) Dongfang Cheng, Ziyang Wei, Zisheng Zhang, Peter Broekmann, Anastassia N. Alexandrova, Philippe Sautet, Restructuring and Activation of Cu(111) under Electrocatalytic Reduction Conditions, Angew. Chem. Int. Ed. 2023, 62, e202218575

409) Nina M. Sackers, Andree Iemhoff, Philippe Sautet, Regina Palkovits, Understanding the structure of isolated iridium sites anchored on a covalent triazine framework, Catal. Sci. Technol., 2023, 13, 2652-2655

410) Nina M. Sackers, Julia Nikodemus, Regina Palkovits, Philippe Sautet, Peter J. C. Hausoul, Ru-Catalyzed Hydrogenolysis of Methanol: A Computational and Kinetics Study, ChemCatChem 2023, 15, e202201530

411) Xiaoyang Fu, Dongfang Cheng, Chengzhang Wan, Simran Kumari, Hongtu Zhang, Ao Zhang, Huaixun Huyan, Jingxuan Zhou, Huaying Ren, Sibo Wang, Zipeng Zhao, Xun Zhao, Jun Chen, Xiaoqing Pan, Philippe Sautet, Yu Huang, Xiangfeng Duan, Bifunctional Ultrathin $RhRu_{0.5}$-Alloy Nanowire Electrocatalysts for Hydrazine-Assisted Water Splitting, Adv. Mater. 2023, 35, 2301533

412) Pallavi Bothra, Adam Z. Stieg, James K. Gimzewski, Philippe Sautet, Controlled Vertical Transfer of Individual Au Atoms Using a Surface Supported Carbon Radical for Atomically Precise Manufacturing, *Precis. Chem.* 2023, 1, 119–126.

413) Robert H. Lavroff, Jason Wang, Michael G. White, Philippe Sautet, Anastassia N. Alexandrova, Mechanism of Stoichiometrically Governed Titanium Oxide Brownian Tree Formation on Stepped Au(111), J. Phys. Chem. C 2023, 127, 8030−8040

414) Celine Tesvara, Christopher J. Karwacki, Philippe Sautet, Decomposition of the Toxic Nerve Agent Sarin on Oxygen Vacancy Sites of Rutile TiO_2(110), J. Phys. Chem. C 2023, 127, 8006−8015

415) Zisheng Zhang, Tsugunosuke Masubuchi, Philippe Sautet, Scott L. Anderson, Anastassia N. Alexandrova, Hydrogen Evolution on Electrode-Supported Ptn Clusters: Ensemble of Hydride States Governs the Size Dependent Reactivity, Angewandte Chemie, 2023, 62, e202218210

416) Zahra Almisbaa, Hassan A. Aljama, Khalid Almajnouni, Luigi Cavallo, and Philippe Sautet, Acetylene Semi-Hydrogenation on Intermetallic Ni−In Catalysts: Ni Ensemble and Acetylene Coverage Effects from a Theoretical Analysis, ACS Catal. 2023, 13, 7358−7370

417) Yichen Li, Dongfang Cheng, Ziyang Wei, and Philippe Sautet, Photoelectron Storage at the WO_3/TiO_2 Interface: Modeling in Ambient Conditions from First-Principles Calculations, ACS Catal. 2023, 13, 9979−9986

418) Kangze Shen, Dongfang Cheng, Eber Reyes-Lopez, Joonbaek Jang, Philippe Sautet, Carlos G. Morales-Guio, On the origin of carbon sources in the electrochemical upgrade of CO_2 from carbon capture solutions, Joule 2023, 7, 1–17.

419) Ziyang Wei, George Yan, Philippe Sautet, Toward more accurate surface properties of ceria using many-body perturbation theory, J. Chem. Phys. 2023, 159, 054708

420) Junjie Shi, Hio Tong Ngan, Philippe Sautet, Jason F. Weaver, High Selectivity and Activity of Ti-Cu(111) Dilute Alloys for the Deoxygenation of Ethanol to Ethylene, ACS Catal. 2023, 13, 11244−11255

421) Selina K. Kaiser, Jessi E. S. van der Hoeven, George Yan, Kang Rui Garrick Lim, Hio Tong Ngan, Sadhya Garg, Mustafa Karatok, Michael Aizenberg, Joanna Aizenberg, Philippe Sautet, Cynthia M. Friend, Robert J. Madix, Identifying the Optimal Pd Ensemble Size in Dilute PdAu Alloy Nanomaterials for Benzaldehyde Hydrogenation, ACS Catal. 2023, 13, 12092−12103

422) Giyeong Son, Yichen Li, Anna V. Shneidman, Jae Hyo Han, Michael Aizenberg, Philippe Sautet, Joanna Aizenberg, Facet-Dependence of Electron Storage in Gold-Decorated Titania Nanocrystals, Chem. Mater. 2023, 35, 9505−9516

423) Simran Kumari, Anastassia N. Alexandrova, Philippe Sautet, Nature of Zirconia on a Copper Inverse Catalyst Under CO_2 Hydrogenation Conditions, J. Am. Chem. Soc. 2023, 145, 26350−26362

424) Alexandre C. Foucher, Hio Tong Ngan, Tanya Shirman, Amanda Filie, Kaining Duanmu, Michael Aizenberg, Robert J. Madix, Cynthia M. Friend, Joanna Aizenberg, Philippe Sautet, Eric A. Stach, Influence of Pd Concentration in Au−Pd Nanoparticles for the Hydrogenation of Alkynes, ACS Appl. Nano Mater. 2023, 6, 22927−22938

425) Hao Chen, Lorenz J. Falling, Heath Kersell, George Yan, Xiao Zhao, Judit Oliver-Meseguer, Max Jaugstetter, Slavomir Nemsak, AdrianHunt, Iradwikanari Waluyo, Hirohito Ogasawara, Alexis T. Bell, Philippe Sautet, Miquel Salmeron, Elucidating the active phases of CoOx films on Au(111) in the CO oxidation reaction, Nature Communications 2023, 14, 6889

426) Rongli Liu, Ziyang Wei, Lele Peng, Leyuan Zhang, Arava Zohar, Rachel Schoeppner, Peiqi Wang, Chengzhang Wan, Dan Zhu, Haotian Liu, Zhaozong Wang, Sarah H. Tolbert, Bruce Dunn, Yu Huang, Philippe Sautet, Xiangfeng Duan, Establishing reaction networks in the 16-electron sulfur reduction reaction, Nature 2024, 626, 98-106

427) Shijia Feng, Xiaojun Wang, Dongfang Cheng, Yao Luo, Mengxin Shen, Jingyang Wang, Wei Zhao, Susu Fang, Hongzhi Zheng, Liyao Ji, Xing Zhang, Weigao Xu, Yongye Liang, Philippe Sautet, Jia Zhu, Stabilizing *CO2 Intermediates at the Acidic Interface using Molecularly Dispersed Cobalt Phthalocyanine as Catalysts for CO_2 Reduction, Angew. Chem. Int. Ed. 2024, 63, e202317942

428) Hio Tong Ngan, Philippe Sautet, Tuning the Hydrogenation Selectivity of an Unsaturated Aldehyde via Single-Atom Alloy Catalysts, J. Am. Chem. Soc. 2024, 146, 2556−2567

429) Dongfang Cheng, Anastassia N. Alexandrova, Philippe Sautet, H‑Induced Restructuring on Cu(111) Triggers CO Electroreduction in an Acidic Electrolyte, J. Phys. Chem. Lett. 2024, 15, 1056−1061

430) Xiaoyang Fu, Dongfang Cheng, Ao Zhang, Jingxuan Zhou, Sibo Wang, Xun Zhao, Jun Chen, Philippe Sautet, Yu Huang, Xiangfeng Duan, Ag–Ru interface for highly efficient hydrazine assisted water electrolysis, Energy Environ. Sci., 2024, 17, 2279

431) Patricia Poths, Santiago Vargas, Philippe Sautet, Anastassia N. Alexandrova, Thermodynamic Equilibrium versus Kinetic Trapping: Thermalization of Cluster Catalyst Ensembles Can Extend Beyond Reaction Time Scales, ACS Catal. 2024, 14, 5403−5415

432) Celine Tesvara, Md Raian Yousuf, Malik Albrahim, Diego Troya, Abhijit Shrotri, Eli Stavitski, Ayman M. Karim, Philippe Sautet, Unraveling the CO Oxidation Mechanism over Highly Dispersed Pt Single Atom on Anatase TiO_2 (101), *ACS Catal.* 2024, 14, 7562–7575

433) Matthew J. Bonney, Celine Tesvara, Philippe Sautet, Michael G. White, Understanding the Decomposition of Dimethyl Methyl Phosphonate on Metal-Modified TiO_2(110) Surfaces Using Ensembles of Product Configurations, *ACS Appl. Mater. Interfaces* 2024, 16, 25483–25497

434) Zisheng Zhang, Winston Gee, Philippe Sautet, Anastassia N. Alexandrova, H and CO Co-Induced Roughening of Cu Surface in CO_2 Electroreduction Conditions, *J. Am. Chem. Soc.* 2024, 146, 16119–16127

435) Sree Harsha Bhimineni, Shu-Ting Ko, Casey Cornwell, Yantao Xia, Sarah H. Tolbert, Jian Luo, Philippe Sautet, First Principles Study of Aluminum Doped Polycrystalline Silicon as a Potential Anode Candidate in Li-ion Batteries, Adv. Energy Mater. 2024, 14, 2400924

436) Mengxin Shen, Liyao Ji, Dongfang Cheng, Ziwei Wang, Qinwen Xue, Shijia Feng, Yao Luo, Shuying Chen, Jiahao Wang, Hongzhi Zheng, Xiaojun Wang, Philippe Sautet, Jia Zhu, Hierarchical design enables sufficient activated CO2 for efficient electrolysis of bicarbonate to CO, Joule 8, 1–17, July 17, 2024
https://doi.org/10.1016/j.joule.2024.04.006

437) Yao Yang, Jihan Zhou, Zipeng Zhao, Geng Sun, Saman Moniri, Colin Ophus, Yongsoo Yang, Ziyang Wei, Yakun Yuan, Cheng Zhu, Yang Liu, Qiang Sun, Qingying Jia, Hendrik Heinz, Jim Ciston, Peter Ercius, Philippe Sautet, Yu Huang, Jianwei Miao, Atomic-scale identification of active sites of oxygen reduction nanocatalysts, Nat. Catal. 2024, 7, 796–806.

438) Robert M. Kowalski, Avishek Banerjee, Chudi Yue, Sara G. Gracia, Dongfang Cheng, Carlos G. Morales-Guio, Philippe Sautet, Electroreduction of Captured CO_2 on Silver Catalysts: Influence of the Capture Agent and Proton Source, *J. Am. Chem. Soc.* 2024, 146, 20728–20741

439) Yani Guan, Justus Kümper, Sonja D. Mürtz, Simran Kumari, Peter J. C. Hausoul, Regina Palkovits, Philippe Sautet, Origin of copper dissolution under electrocatalytic reduction conditions involving amines, Chem. Sci., 2024, 15, 14485

440) Hua An, Yani Ding, Philippe Sautet, Geng Sun, Ning Yan, Selective Reduction of Nitroarenes via Noncontact Hydrogenation, *J. Am. Chem. Soc.* 2024, 146, 29315–29324

441) Zahra Almisbaa, Philippe Sautet, Ba promoter effect on cobalt-catalyzed ammonia decomposition kinetics: A theoretical analysis, Journal of Energy Chemistry 2024, 99, 182–192

442) Justus Kümper, Sonja D. Mürtz, Yani Guan, Simran Kumari, Peter J. C. Hausoul, Nils Kurig, Philippe Sautet, Regina Palkovits, Metallic Impurities in Electrolysis: Catalytic Effect of Pb Traces in Reductive Amination and Acetone Reduction, *Angew. Chem. Int. Ed.* 2024, 63, e202411532

443) Xintong Yuan, Dongfang Cheng, Bo Liu, Kaiyan Liang, Keyue Liang, JiayiYu, Matthew Mecklenburg, Philippe Sautet, Yuzhang Li, Engineering battery corrosion films by tuning electrical double layer composition, Joule 2024, 8, 3038 – 3053

444) Yu Tang, George Yan, Shiran Zhang, Yuting Li, Luan Nguyen, Yasuhiro Iwasawa, Tomohiro Sakata, Christopher Andolina, Judith C. Yang, Philippe Sautet, Franklin Feng Tao, Turning on Low-Temperature Catalytic Conversion of Biomass Derivatives through Teaming Pd1 and Mo1 Single-Atom Sites, Nat. Catal. 2024, 7, 796–806

445) Robert H. Lavroff, Edison Cummings, Kaustubh Sawant, Zisheng Zhang, Philippe Sautet, Anastassia N. Alexandrova, Cu-Supported ZnO under Conditions of CO_2 Reduction to Methanol: Why 0.2 ML Coverage?, J. Phys. Chem. Lett. 2024, 15, 11745−11752

446) Yani Guan, Justus Kümper, Simran Kumari, Nick Heiming, Sonja D. Mürtz, Stephan N. Steinmann, Stefan Palkovits, Regina Palkovits, Philippe Sautet, Probing the Electric Double-Layer Capacitance to Understand the Reaction Environment in Conditions of Electrochemical Amination of Acetone, ACS Appl. Mater. Interfaces 2025, 17, 4087−4097

447) Zahra Almisbaa, Philippe Sautet, Effect of water impurities on promoted and unpromoted cobalt-catalysts during the ammonia decomposition reaction, Journal of Catalysis, 2025, 446, 116054.

448) Dongfang Cheng, Ziyang Wei, Philippe Sautet, Elucidating the Proton Source for CO_2 Electro-Reduction on Cu(100) Using Many-Body Perturbation Theory, Journal of the American Chemical Society 2025 147, 10954-10965

449) Avik Halder, Robert E. Warburton, Geng Sun, Lei Cheng, Rajeev S. Assary, Soenke Seifert, Micaela Homer, Jeffrey Greeley, Anastassia N. Alexandrova, Philippe Sautet, Larry A. Curtiss, and Stefan Vajda, Low-Temperature Direct Oxidation of Propane to Propylene Oxide Using Supported Subnanometer Cu Clusters, *ACS Catalysis* **2025** *15* (7), 5760-5769

450) Prahlad K. Routh, Xihan Liu, Evgeniy Redekop, Jin Soo Lim, Sebastian Prodinger, Jessi E. S. van der Hoeven, Joanna Aizenberg, Maarten Nachtegaal, Adam H. Clark, Philippe Sautet, and Anatoly I. Frenkel, Unraveling the Kinetics of Hydride Formation and

Decomposition at Pd–Au Bimetallic Interfaces: A Combined Spectroscopic and Computational Study, *Journal of the American Chemical Society* **2025** *147* (13), 11378-11389

451) Yicheng Wang, Hio Tong Ngan, Ho-Yi Lam, George Yan, Ryan T. Hannagan, Volkan Çınar, Nathaniel M. Eagan, Prashant Deshlahra, Philippe Sautet, and E. Charles H. Sykes, Direct Comparison of the Activity and Selectivity of Rh_1Cu and Ni_1Cu Single-Atom Alloy Sites for Ethanol Decomposition, *ACS Catalysis* **2025** *15* (8), 6046-6057

452) Zihan Yang, Simran Kumari, Anastassia N. Alexandrova, Philippe Sautet, Catalytic Activity of an Ensemble of Sites for CO_2 Hydrogenation to Methanol on a ZrO_2-on-Cu Inverse Catalyst, J. Am. Chem. Soc. 2025, 147, 18, 15294–15306

453) Cheng, D., Nguyen, KL.C., Sumaria, V., Ziyang Wei, Zisheng Zhang, Winston Gee, Yichen Li, Carlos G. Morales-Guio, Markus Heyde, Beatriz Roldan Cuenya, Anastassia N. Alexandrova& Philippe Sautet, Structure Sensitivity and Catalyst Restructuring for CO_2 Electro-reduction on Copper. Nat Commun 16, 4064 (2025)

454) Robert Michael Kowalski, Dongfang Cheng, Philippe Sautet, A tutorial on the modeling of the heterogenous captured CO_2electroreduction reaction and first principles electrochemical modeling, Chem. Soc. Rev., 2025,54, 5766-5791

455) Huida Lyu, Jung Tae Kim, Dongfang Cheng, Xintong Yuan, Mackenzie Anderson, Keyue Liang, Jiayi Yu, Philippe Sautet, Richard Kaner, and Yuzhang Li, Localized Eutectic Electrolytes for Stable Aqueous Zinc-Ion Batteries, *ACS Energy Letters* **2025** *10* (6), 2924-2933

456) Fu, X., Cheng, D., Zhang, A., Zhou, J., Wang, S., Wan, C., Zhao, X., Chen, J., Sautet, P., Huang, Y. and Duan, X. (2025), High-Performance Cu_6Sn_5 Alloy Electrocatalysts for Formaldehyde Oxidative Dehydrogenation and Bipolar Hydrogen Production. Angew. Chem. Int. Ed., 64: e202503828.

457) Sree Harsha Bhimineni and Philippe Sautet, Formation of Solid Electrolyte Interphase from the Decomposition of Ethylene Carbonate on Aluminum-Doped Silicon - A DFT Analysis, ACS Applied Energy Materials 2025 8 (13), 8887-8895

458) K. J. Sawant, D. Stockwell, A. Debellis, L. Dorazio, P. Sautet, Ensemble of Active Acid Sites on Amorphous Silica–Alumina Surfaces for Catalytic Cracking, *Angew. Chem. Int. Ed.* 2025, 64, e202506711.

459) Gong Zhang, Lee Fuller, Christine Lucky, Alexander J. Zielinski, Dongfang Cheng, Enner Mendoza, Philippe Sautet, and Marcel Schreier, Room-Temperature Electrocatalytic Dehydrogenation and Partial Fragmentation of *n*-Alkanes, *Journal of the American Chemical Society* **2025** *147* (39), 35219-35226