

## List of Publications

1. O. Gropen, U. Wahlgren and L. Pettersson, *Effective Core Potential Calculations on the  $[NiH_4]^{2-}$  ion as a Testcase for Studying Rotational Barriers*, Chem. Phys. **66**, 453 (1982).
2. O. Gropen, U. Wahlgren and L. Pettersson, *Effective Core Potential Calculations on Small Molecules Containing Transition Metal Atoms*, Chem. Phys. **66**, 459 (1982).
3. L. Pettersson and U. Wahlgren, *An Investigation of Basis Sets and Basis Set Superposition Error in Transition Metals Using Frozen Core and Frozen Orbital Techniques*, Chem. Phys. **69**, 185 (1982).
4. L. Pettersson and U. Wahlgren, *Investigation of Heavily Contracted Basis Sets and Superposition Errors for some First and Second Row Transition Elements*, Chem. Phys. Letters **89**, 26 (1982).
5. S. Ollmar and L. Pettersson, *Patterns of Electrical Parameters in Fertilized and Unfertilized Hens' Eggs*, USIP Report 82-07.
6. L.G.M. Pettersson, P.E.M. Siegbahn and O. Gropen, *The Binding in  $ClF_3$* , Mol. Phys. **48**, 871 (1983).
7. M. Blomberg, U. Brandemark, L. Pettersson and P. Siegbahn, *Contracted CI Calculations of Models for Catalytic Reactions Involving Transition Metals*, Int. J. Quant. Chem. **XXIII**, 855 (1983).
8. L.G.M. Pettersson, U. Wahlgren and O. Gropen, *Effective Core Potential Calculations Using Frozen Orbitals. Applications to Transition Metals*, Chem. Phys. **80**, 7 (1983).
9. L.G.M. Pettersson, P.E.M. Siegbahn and S. Ismail, *Core Valence Correlation Effects in Calcium Hydride*, Chem. Phys. **82**, 355 (1983).
10. L.G.M. Pettersson and A. Strömberg, *A Study of the Valence Interaction Integrals in Effective Core Potential Applications*, Chem. Phys. Letters **99**, 122 (1983).
11. M. Blomberg, U. Brandemark, L. Pettersson, P. Siegbahn and M. Larsson, *The CASSCF and Contracted CI Methods Applied to Three Different Chemical Problems*, Proceedings of the CCP1 Study Weekend, March 1983, edited by R.D. Amos and M.F. Guest.
12. U. Brandemark, M.R.A. Blomberg, L.G.M. Pettersson and P.E.M. Siegbahn, *Theoretical Investigation of the Addition of Molecular Hydrogen to Pd and  $(H_2O)_2Pd$* , J. Phys. Chem. **88**, 4617 (1984).
13. L. Pettersson, *Studies in Molecular Structure and Bonding Using Effective Core Potential and Accurate CI Methods*, Doctoral Thesis, ISBN-91-7146-287-2, Stockholm University, 1984.
14. E. Björkman, L. Pettersson, P. Siegbahn and J. Bäckwall, *Reactivity of Coordinated Nucleophile towards cis-Migration in ( $\pi$ -olefin)Palladium Complexes*, J. Am. Chem. Soc. **106**, 4369 (1984).

15. P.O. Jansson, L. Pettersson and U. Wahlgren, *Matrix Induced Effects on the A-X and E-X Transitions in SiO. A Theoretical Study*, Chem. Phys. **85**, 355 (1984).
16. K. Broch Mathisen, L.G.M. Pettersson and U. Wahlgren, *CASSCF Calculations Using Effective Core Potentials on the Optical Spectrum of Mo<sub>2</sub>Cl<sub>8</sub><sup>4-</sup>*, Chem. Phys. Letters **104**, 336 (1984).
17. A. Strömberg, U. Wahlgren, L. Pettersson and P. Siegbahn, *On the Role of 3d orbitals in Sulfur*, Chem. Phys. **89**, 323 (1984).
18. M. Arbman, H. Siegbahn, L. Pettersson and P. Siegbahn, *Core Electron Binding Energies and Auger Electron Energies of Solvated Clusters. A Computational Study*, Mol. Phys. **54**, 1149 (1985).
19. L.G.M. Pettersson and P.E.M. Siegbahn, *The Effect of 3d Shell Backbonding on the Binding of Chlorine Containing Molecules*, J. Chem. Phys. **83**, 3538 (1985).
20. A. Strömberg, L. Pettersson and U. Wahlgren, *CASSCF ECP Calculations on the Optical Spectrum of Mo<sub>2</sub>(O<sub>2</sub>CH)<sub>4</sub> and on the Barrier to Internal Rotation in Mo<sub>2</sub>Cl<sub>8</sub><sup>4-</sup>*, Chem. Phys. Letters **118**, 389 (1985).
21. E.E. Björkman, L. Pettersson, P. Siegbahn and J.E. Bäckwall, *A Theoretical Study on the Reactivity of Nucleophiles Coordinated to Palladium*, J. Am. Chem. Soc. **107**, 7265 (1985).
22. J.E. Bäckwall, E.E. Björkman, L. Pettersson, P. Siegbahn and A. Strich, *A Theoretical Study of the Cyclopropane Ring-Opening by Palladium*, J. Am. Chem. Soc. **107**, 7408 (1985).
23. C.W. Bauschlicher and L.G.M. Pettersson, *The Structure of Small Metal Clusters*, IBM RJ 4812 (50963) 8/26/85, J. Chem. Phys. **84**, 2226 (1986).
24. L.G.M. Pettersson and P.S. Bagus, *Adsorbate Ionicity and Surface Dipole Moment Changes; Cluster Model Studies of Cl/Cu(100) and F/Cu(100)*, IBM RJ 4812 (50963) 9/5/85, Phys. Rev. Letters **56**, 500 (1986).
25. L.G.M. Pettersson and P.E.M. Siegbahn, *Accurate Effective Core Potential for Germanium. Application to the Singlet-Triplet Splitting in GeH<sub>2</sub>*, Chem. Phys. **105**, 355 (1986).
26. L.G.M. Pettersson, C.W. Bauschlicher and I. Hussla, *Vibrations of Ammonia on the Cu(100) Surface*, J. Vac. Science and Technology A **4**, 1470 (1986).
27. L.G.M. Pettersson and S.R. Langhoff, *Theoretical Electric Dipole Moments of SiH, GeH and SnH*, Chem. Phys. Letters **125**, 429 (1986).
28. L.G.M. Pettersson, S.R. Langhoff and D. Chong, *Theoretical Study of the Electric Dipole Moment Function of the ClO Molecule*, J. Chem. Phys. **85**, 2836 (1986).
29. L.G.M. Pettersson and S.R. Langhoff, *Theoretical Electric Dipole Moments and Dissociation Energies for the Ground States of GaH - BrH*, J. Chem. Phys. **85**, 3130 (1986).

- 30.** L.G.M. Pettersson and C.W. Bauschlicher, *Stability and Structure of Metal Clusters: Be<sub>13</sub> – Be<sub>55</sub>*, Chem. Phys. Letters **130**, 111 (1986).
- 31.** S.R. Langhoff, L.G.M. Pettersson, C.W. Bauschlicher, and H. Partridge, *Theoretical spectroscopic parameters for the low-lying states of the second-row transition metal hydrides*, J. Chem. Phys. **86**, 268 (1987).
- 32.** C.W. Bauschlicher, Jr, L.G.M. Pettersson, *Small Al clusters I: The effect of basis set and correlation on the geometry of small Al clusters*, J. Chem. Phys. **87**, 2198 (1987).
- 33.** L.G.M. Pettersson, C.W. Bauschlicher and T. Halicioglu, *Small Al clusters II: Structure and binding in Al<sub>n</sub> (n=2-6,13)*, J. Chem. Phys. **87**, 2205 (1987).
- 34.** L.G.M. Pettersson, U. Wahlgren and O. Gropen, *Effective Core Potential Parameters for the First and Second Row Atoms*, J. Chem. Phys. **86**, 2176 (1987).
- 35.** C.W. Bauschlicher, L.G.M. Pettersson, and Per E.M. Siegbahn, *The bonding in FeN<sub>2</sub>, FeCO and Fe<sub>2</sub>N<sub>2</sub>: Model systems for side-on bonding of CO and N<sub>2</sub>*, J. Chem. Phys. **87**, 2129 (1987).
- 36.** L.G.M. Pettersson, S.R. Langhoff, C.W. Bauschlicher, and H. Partridge, *Positive ions of the first- and second-row transition metal hydrides*, J. Chem. Phys. **87**, 481 (1987).
- 37.** P. Bowen-Jenkins, L.G.M. Pettersson, P. Siegbahn, J. Almlöf and P.R. Taylor, *The bond distance in methane*, J. Chem. Phys. **88**, 6977 (1988).
- 38.** C.W. Bauschlicher, P. Siegbahn and L.G.M. Pettersson, *The atomic states of nickel*, Theor. Chim. Acta **74**, 479 (1988).
- 39.** H. Åkeby and L.G.M. Pettersson, *Low-lying Singlet States of MgCl<sup>+</sup>*, Chem. Phys. Letters **146**, 511 (1988).
- 40.** C.W. Bauschlicher, S.R. Langhoff and L.G.M. Pettersson, *The Computed Spectrum of AlC*, J. Chem. Phys. **89**, 5747 (1988).
- 41.** S.R. Langhoff, C.W. Bauschlicher and L.G.M. Pettersson, *Theoretical spectrum of AlN*, J. Chem. Phys. **89**, 7354 (1988).
- 42.** S.R. Langhoff, C.W. Bauschlicher, L.G.M. Pettersson and P.E.M. Siegbahn, *Theoretical Spectroscopic Parameters for the Low-lying States of the Oxides and Sulfides of Mo and Tc*, Chem. Phys. **132**, 49 (1989).
- 43.** B. Beagley, A. Eriksson, J. Lindgren, I. Persson, L. Pettersson, M. Sandström, U. Wahlgren and E.W. White, *A computational and experimental-study on the Jahn-Teller effect in the hydrated copper(II) ion - comparisons with hydrated nickel(II) ions in aqueous-solution and solid Tuttons salts*, Journal of Physics: Condensed Matter **1**, 2395 (1989).
- 44.** L.G.M. Pettersson and C.W. Bauschlicher, *The Effect of Impurities on the Structure of Small Al and Be Clusters*, Chem. Phys. **131**, 267 (1989).

- 45.** U. Wahlgren, L.G.M. Pettersson, and P. Siegbahn, *Cu 3d covalency in chemisorption?*, J. Chem. Phys. **90**, 4613 (1989).
- 46.** L.G.M. Pettersson, P. Siegbahn, H. Åkeby, and U. Wahlgren, *Large-Scale Computations on Three Quantum Chemical Problems, Proceedings of the Workshop on Supercomputing Tools for Science and Engineering*, Pisa, Italy, December 4-7, 1989.
- 47.** H. Partridge, C.W. Bauschlicher, L.G.M. Pettersson, A.D. Maclean, B. Liu, M. Yoshimine, and A. Komornicki, *On the dissociation energy of Mg<sub>2</sub>*, J. Chem. Phys. **92**, 5377 (1990).
- 48.** H. Åkeby, I. Panas, L.G.M. Pettersson, P. Siegbahn, and U. Wahlgren, *The electronic and geometric structure of the Cu<sub>n</sub> cluster anions, n≤10*, J. Phys. Chem. **94**, 5471 (1990).
- 49.** L.G.M. Pettersson, H. Åkeby, P. Siegbahn and U. Wahlgren, *The Effects of Core(3d) Correlation on Chemisorption*, J. Chem. Phys **93**, 4954 (1990).
- 50.** L.G.M. Pettersson and J. Schüle, *Singlet-Triplet Separation in Some GeXY (X,Y=H,Li,F) Compounds*, J. Mol. Struct. (THEOCHEM) **208**, 137 (1990).
- 51.** L.G.M. Pettersson and H. Åkeby, *Core-valence correlation effects using approximate operators*, J. Chem. Phys. **94**, 2968 (1991).
- 52.** L.G.M. Pettersson and M. Larsson, *On the Character of the O<sub>2</sub><sup>2+</sup> A 3Σ<sub>u</sub><sup>+</sup> State*, J. Chem. Phys. **94**, 818 (1991).
- 53.** K. Børve and L.G.M. Pettersson, *Gasphase Hydrogen Abstraction from Methane Using Metal Oxides. Theoretical Study*, J. Phys. Chem. **95**, 3214 (1991).
- 54.** H. Åkeby and L.G.M. Pettersson, *Core-valence Correlation Effects on some Cu Clusters*, Chem. Phys. **155**, 197 (1991).
- 55.** K. Børve and L.G.M. Pettersson, *Hydrogen Abstraction from Methane on the MgO(001) Surface*, J. Phys. Chem. **95**, 7401 (1991).
- 56.** P.E.M. Siegbahn, L.G.M. Pettersson and U. Wahlgren, *A Theoretical Study of Atomic Fluorine Chemisorption on the Ni(100) Surface*, J. Chem. Phys. **94**, 4024 (1991).
- 57.** L.G.M. Pettersson, *Large Atomic Core-Core Correlation Effects*, Chem. Phys. Letters **180**, 365 (1991).
- 58.** R. Åkesson, L.G.M. Pettersson, M. Sandström and U. Wahlgren, *Theoretical Calculations of the Jahn-Teller Effect in the hexahydrated copper(II), chromium(II) and manganese(III) ions, [Cu(H<sub>2</sub>O)<sub>6</sub>]<sup>2+</sup>, [Cr(H<sub>2</sub>O)<sub>6</sub>]<sup>2+</sup> and [Mn(H<sub>2</sub>O)<sub>6</sub>]<sup>3+</sup>, and comparisons with the hexahydrated copper(I), chromium(III), and manganese(II) clusters*, J. Phys. Chem. **96**, 150 (1992).
- 59.** L.G.M. Pettersson, L. Karlsson, M.P. Keane, A. Naves de Brito, N. Correia, M. Larsson, L. Broström, S. Mannervik and S. Svensson, *The X-ray excited Auger electron spectrum of NO and potential curves for the NO<sup>2+</sup> ion*, J. Chem. Phys. **96**, 4884 (1992).

- 60.** F. Bökman, A. Gogoll, L.G.M. Pettersson, O. Bohman and H. Siegbahn, *Electronic Structure of Catalytically Important Palladium Complexes Studied by Photoelectron Spectroscopy*, Organometallics **11**, 1784 (1992).
- 61.** L.G.M. Pettersson, P.E.M. Siegbahn, L. Broström, S. Mannervik and M. Larsson, *Theoretical Potential Curves for the  $A\ ^2\Pi$  and  $X\ ^2\Sigma^+$  States of  $NO^{2+}$  and an Experimental Search for the A-X Transition*, Chem. Phys. Letters **191**, 279 (1992).
- 62.** M.A. Nygren and L.G.M. Pettersson, *The structure and spectrum of the  $C_4$  molecule*, Chem. Phys. Letters **191**, 473 (1992).
- 63.** H. Åkeby, L.G.M. Pettersson, and P.E.M. Siegbahn, *Core-Correlation and the Binding Energy of  $Sc_2$* , J. Chem. Phys. **97**, 1850 (1992).
- 64.** R. Åkesson, M. Sandström, L.G.M. Pettersson, P.E.M. Siegbahn and U. Wahlgren, *Theoretical Ab Initio SCF Study of Binding Energies and Ligand Field Effects for the Hexahydrated Divalent Ions of the First-Row Transition Metals*, J. Phys. Chem. **96**, 10773 (1992).
- 65.** L.G.M. Pettersson and T. Faxén, *Massively Parallelized Direct SCF Calculations on Large Metal Clusters:  $Ni_5 - Ni_{481}$* , Theoret. Chim. Acta **85**, 345 (1993).
- 66.** R. Åkesson, M. Sandström, L.G.M. Pettersson, P.E.M. Siegbahn and U. Wahlgren, *Theoretical Study of Water Exchange Reactions for the Divalent Ions of the First Transition Period*, J. Phys. Chem. **97**, 3765 (1993).
- 67.** H. Åkeby and L.G.M. Pettersson, *Partition Function and Dissociation Energy for  $Sc_2X\ ^5\Sigma_u^-$* , J. Mol. Spect. **159**, 17 (1993).
- 68.** J. Persson and L.G.M. Pettersson, *Effects of core correlation on atomic and dimeric phosphorus*, Chem. Phys. **170**, 149 (1993).
- 69.** C.W. Bauschlicher Jr, H. Partridge and L.G.M. Pettersson, *Franck-Condon factors for photodetachment from  $LiO^-$ ,  $NaO^-$ , and  $KO^-$* , J. Chem. Phys. **99**, 3654 (1993).
- 70.** L. Seijo, Z. Barandiarán and L.G.M. Pettersson, *Ab initio model potential study of pressure effects on  $K_2NaGaF_6:Cr^{3+}$* , J. Chem. Phys. **98**, 4041 (1993).
- 71.** K. Hermann, M. Wittko, L.G.M. Pettersson and P.E.M. Siegbahn, *Binding of radical species to metal surfaces: Cluster models for OH on Cu(111)*, J. Chem. Phys. **99**, 610 (1993).
- 72.** L.G.M. Pettersson and H. Holmgren, *Aspects and Applications of Computers in Chemistry, Proceedings of the First National Vietnamese Seminar on Informatics Applied to Chemistry*, Hanoi 28-29/7 1993.
- 73.** C. Ribbing, M. Odelius, J. Kowalewski, and L.G.M. Pettersson, *Simple non-empirical calculations of the zero-field splitting in bis(aquo)bis(malonato) nickel(II)*, Theoret. Chim. Acta **87**, 307 (1994).
- 74.** M. Nygren, L.G.M. Pettersson, Z. Barandiarán, and L. Seijo, *Bonding between CO and the  $MgO(001)$  surface - A modified picture*, J. Chem. Phys. **100**, 2010 (1994).

75. J. Olsen, L.G.M. Pettersson and D. Sundholm, *Calculations of excitation energies and electron affinities for Be*, J. Phys. **B27**, 5575 (1994).
76. L.G.M. Pettersson, *The bonding between NO and the NiO(100) surface*, Theoret. Chim. Acta **87**, 293 (1994).
77. R. Åkesson, L.G.M. Pettersson, M. Sandström, and U. Wahlgren, *Ligand Field Effects in the Hydrated Divalent and Trivalent Metal Ions of the First and Second Transition Periods*, J. Am. Chem. Soc. **116**, 8691 (1994).
78. L.G.M. Pettersson and G. Pacchioni, *The Electronic Structure of an Oxygen Defect in NiO(100)*, Chem. Phys. Letters **219**, 107 (1994).
79. R. Åkesson and L.G.M. Pettersson, *Theoretical Study of the Mono- and Dihydrated Dipositive Ions of the First-Row Transition Metals*, Chem. Phys. **184**, 85 (1994).
80. M.A. Nygren and L.G.M. Pettersson, *Adsorption of Small Molecules on Metal Oxides*, J. Electr. Spect. Rel. Phen. **69**, 43 (1994).
81. R. Åkesson, L.G.M. Pettersson, M. Sandström, and U. Wahlgren, *Theoretical Study on Water-Exchange Reactions of the Divalent and Trivalent Metal Ions of the First Transition Period*, J. Am. Chem. Soc. **116**, 8705 (1994).
82. M.A. Nygren and L.G.M. Pettersson, *Theoretical modeling of metal-oxides - influence of field-strength on Atomic Oxygen Adsorption and a Simple Model Reaction: O<sub>ads</sub>+CO→CO<sub>2</sub>*, Chem. Phys. Letters **230**, 456 (1994).
83. H. Ågren, V. Caravetta, O. Vahtras, and L.G.M. Pettersson, *Direct, Atomic Orbital, Static Exchange Calculations of Photoabsorption Spectra of Large Molecules and Clusters*, Chem. Phys. Letters **222**, 75 (1994).
84. L.A. Eriksson, L.G.M. Pettersson, P.E.M. Siegbahn and U. Wahlgren, *On the Accuracy of Gradient Corrected Density Functional Methods for Transition Metal Complexes*, J. Chem. Phys. **102**, 872 (1995).
85. V. Caravetta, H. Ågren, L.G.M. Pettersson and O. Vahtras, *Near-Edge Core Photoabsorption in Polyenes*, J. Chem. Phys. **102**, 5589 (1995).
86. H. Ågren, V. Caravetta, L.G.M. Pettersson and O. Vahtras, *Static Exchange Calculations of X-ray Absorption Fine Structures in Polymers and Surface Adsorbates*, Physica B – Cond. Mat. **209**, 477 (1995).
87. Hans Ågren, Vincenzo Caravetta, Olav Vahtras and Lars G.M. Pettersson, *On the orientational probing of polymeric thin films by NEXAFS. Calculations on poly-tetrafluoroethylene*, Phys. Rev. B: Conden. Matter **51**, 17848 (1995).
88. Lars G.M. Pettersson, Hans Ågren, Olav Vahtras and Vincenzo Caravetta, *Calculation of NEXAFS Spectra for Adsorbates: OH/Cu(111)*, J. Chem. Phys. **103**, 8713 (1995).

- 89.** M. Schönenbeck, D. Cappus, J. Klinkmann, H.-J. Freund, L.G.M. Pettersson, and P.S. Bagus, *Adsorption of CO and NO on NiO and CoO: a comparison*, Surface Science **347**, 337 (1996).
- 90.** M.A. Nygren, L.G.M. Pettersson, A. Freitag, V. Staemmler, D.H. Gay and A.L. Rohl, *Theoretical Models of the Polar Cu<sub>2</sub>O(100) Cu<sup>+</sup>-terminated Surface*, J. Phys. Chem. **100**, 294 (1996).
- 91.** Martin A. Nygren and Lars G.M. Pettersson, *H<sub>2</sub>O interaction with the polar Cu<sub>2</sub>O(100) surface: A theoretical study*, J. Phys. Chem. **100**, 1874 (1996).
- 92.** Vincenzo Carravetta, Lars G.M. Pettersson, Olav Vahtras and Hans Ågren, *Self-consistent Field Calculations of X-ray Emission Spectra of Surface Adsorbates: CO/Cu(100)*, Surf. Sci. **369**, 146 (1996).
- 93.** Lars G.M. Pettersson, Hans Ågren, Olav Vahtras and Vincenzo Carravetta, *Cluster Modelling of Core Electron Photoabsorption of CO Adsorbed on Cu(100)*, Surf. Sci. **365**, 581 (1996).
- 94.** Hans Ågren, Vincenzo Carravetta, Lars G.M. Pettersson and Olav Vahtras, *Static Exchange and Cluster Modelling of Core Electron Shake-up Spectra of Surface Adsorbates: CO/Cu(100)*, Phys. Rev. B **53**, 16074 (1996).
- 95.** Mats Nyberg, Martin A. Nygren, Lars G.M. Pettersson, David H. Gay and Andrew Rohl, *Hydrogen Dissociation on Reconstructed ZnO Surfaces*, J. Phys. Chem. **100**, 9054 (1996).
- 96.** Li Yang, Hans Ågren, Vincenzo Carravetta and Lars G.M. Pettersson, *Static Exchange and Quantum Defect Analysis of X-ray Absorption Spectra of Carbonyl Compounds*, Physica Scripta **54**, 614 (1996).
- 97.** Luciano Triguero, Ulf Wahlgren, Lars G.M. Pettersson and Per Siegbahn, *DFT and MO Calculations of Atomic and Molecular Chemisorption Energies on Surface Cluster Models*, Theoretica Chimica Acta **94**, 297 (1996).
- 98.** Martin A. Nygren and Lars G.M. Pettersson, *Comparing Ab Initio Computed Energetics with Thermal Experiments in Surface Science*, J. Chem. Phys. **105**, 9339 (1996).
- 99.** Lars G.M. Pettersson, *New Developments and Aspects of Computational Chemistry, Proceedings of the Second National Vietnamese Seminar on Informatics Applied to Chemistry*, Hanoi 2-3/5 1996.
- 100.** Vincenzo Carravetta, Hans Ågren, Li Yang and Lars G.M. Pettersson, *On the interpretation of the NEXAFS spectrum of molecular oxygen*, Chem. Phys. Letters **259**, 21 (1996).
- 101.** L.G.M. Pettersson, H. Ågren, B.L. Schürmann, A. Lippitz and W.E.S. Unger, *Assembly and decomposition of building blocks to analyze polymer NEXAFS spectra*, Int. J. Quantum Chem. **63**, 749 (1997).
- 102.** H. Strandh, L.G.M. Pettersson, L. Sjöberg and U. Wahlgren, *Quantum Chemical Studies of the Effect on Silicate Mineral Dissolution Rates by Adsorption of Alkali Metals*, Geochimica and Cosmochimica Acta **61**, 2577 (1997).

- 103.** Li Yang, Hans Ågren, Lars G.M. Pettersson and Vincenzo Carravetta, *On the initial and final state rules for predicting near-edge X-ray absorption intensities*, J. Electron Spect. and Related Phen. **83**, 209 (1997).
- 104.** José-Luis Pascual and Lars G.M. Pettersson, *Electrostatic Potential from Embedded Clusters*, Chem. Phys. Letters **270**, 351 (1997).
- 105.** Lars G.M. Pettersson, Martin A. Nygren, Mats Nyberg and José-Luis Pascual, *Theoretical Modelling of Chemisorption and Reactions on Metal-Oxide Surfaces*, in G. Pacchioni and R.M. Lambert, Editors: *Chemisorption and Reactivity on Supported Clusters and Thin Films: Towards an Understanding of Microscopic Processes in Catalysis*, Kluwer Academic Publishers, Dordrecht, Holland (1997).
- 106.** L. Yang, O. Plachkevych, H. Ågren and L.G.M. Pettersson, *Calculations of NEXAFS spectra of substituted benzenes*, J. Phys. IV France **7**, C2-217 (1997).
- 107.** H. Ågren, L.G.M. Pettersson, V. Carravetta, Y. Luo, L. Yang and O. Vahtras, *Self-Consistent field calculations of X-ray emission spectra of surface adsorbates and polymers*, J. Phys. IV France **7**, C2-515 (1997).
- 108.** V. Carravetta, L. Yang, O. Vahtras, H. Ågren and L.G.M. Pettersson, *Ab-initio static exchange calculations of shake-up spectra of molecules and surface adsorbates*, J. Phys. IV France **7**, C2-519 (1997).
- 109.** H. Ågren, V. Carravetta, O. Vahtras and L.G.M. Pettersson, *Direct SCF - Direct Static Exchange Calculations of Electronic Spectra*, Theoretical Chemistry Accounts **97**, 14 (1997).
- 110.** J.-L. Pascual, L.G.M. Pettersson and H. Ågren, *A Theoretical Study of the UPS Spectra of Carbonyl Systems: CO, Cr(CO)<sub>6</sub> and CO/Cu(100)*, Phys Rev B **56**, 7716 (1997).
- 111.** O. Plashkevych, L. Yang, O. Vahtras, H. Ågren and L.G.M. Pettersson, *Substituted benzenes as building blocks in NEXAFS*, Chem. Phys. **222**, 125 (1997).
- 112.** L. Triguero and L.G.M. Pettersson, *MO and DFT Approaches to the Calculation of X-ray Absorption/Emission Spectra of Nitrogen Atom Adsorbed on Cu(100)*, Surf. Sci. **398**, 70 (1998).
- 113.** P. Bennich, A. Nilsson, T. Wiell, O. Karis, M. Weinelt, N. Wassdahl, M. Nyberg, L.G.M. Pettersson, J. Stöhr and M. Samant, *The nature of the surface chemical bond in N<sub>2</sub> on Ni(100) studied by X-ray emission spectroscopy and ab initio calculations*, Phys. Rev. B **57**, 9274 (1998).
- 114.** C. Focsa, M. Bencheikh and L.G.M. Pettersson, *The electronic structure of TiCl: ligand field versus density functional calculations*, J. Phys. B **31**, 2857 (1998).
- 115.** J. Hasselström, O. Karis, M. Weinelt, N. Wassdahl, A. Nilsson, M. Nyberg, L.G.M. Pettersson, M.G. Samant and J. Stöhr, *The adsorption structure of glycine adsorbed on Cu(110); Comparison to acetate/Cu(110)*, Surf. Sci. **407**, 221 (1998).

- 116.** L. Triguero, L.G.M. Pettersson, B. Minaev and H. Ågren, *Spin Uncoupling in Surface Chemisorption of Unsaturated Hydrocarbons*, J. Chem. Phys. **108**, 1193 (1998).
- 117.** L.G.M. Pettersson, H. Ågren, Y. Luo, L. Triguero, *Benzene Adsorbed on Cu(110): Theoretical X-ray Absorption, Emission and Shake Calculations*, Surf. Sci. **408**, 1 (1998).
- 118.** L. Triguero, L.G.M. Pettersson and H. Ågren, *Calculations of Near-Edge X-ray Absorption Spectra of Gas Phase and Chemisorbed Molecules by means of Density Functional and Transition Potential Theory*, Phys. Rev. B **58**, 8097 (1998).
- 119.** M.-H. Schaffner, F. Patthey, W.-D. Schneider and L.G.M. Pettersson, *Electron Energy Loss Spectroscopy (EELS) of Thermally Evaporated Cu and Small Size-selected Cu Clusters Deposited on MgO(100)/Mo(100)*, Surface Science **402/404**, 450 (1998).
- 120.** L. Triguero, L.G.M. Pettersson and H. Ågren, *Calculations of X-ray Emission Spectra of Molecules and Surface Adsorbates by Means of Density Functional Theory*, J. Phys. Chem. A, **102**, 10599 (1998).
- 121.** L. Triguero, Y. Luo, L.G.M. Pettersson, H. Ågren, P. Väterlein, M. Weinelt, A. Föhlisch, J. Hasselström, O. Karis and A. Nilsson, *Resonant soft X-ray emission spectroscopy of surface adsorbates: Theory, computations and measurements of ethylene and benzene on Cu(110)*, Phys. Rev. B **59**, 5189 (1999).
- 122.** J. Hasselström, A. Föhlisch, O. Karis, M. Weinelt, N. Wassdahl, A. Nilsson, M. Nyberg, L.G.M. Pettersson, M.G. Samant and J. Stöhr, *Ammonia adsorbed on Cu(110): An angle resolved X-ray emission and ab initio study*, J. Chem. Phys. **110**, 4880 (1999).
- 123.** Li Yang, Hans Ågren, Lars G.M. Pettersson, Jinghua Guo, Conny Såthe, Alexander Föhlisch, Anders Nilsson, and Joseph Nordgren, *Core electron spectroscopy of chromium hexacarbonyl. A comparative theoretical and experimental study*, Physica Scripta **59**, 138 (1999).
- 124.** Stefano de Carolis, José Luis Pascual, Lars G.M. Pettersson, Micael Baudin, Mark Wójcik, Kersti Hermansson, Anders Palmqvist and Mamoun Mohammed, *Structure and Electronic Properties of Ca-doped CeO<sub>2</sub>: An Experimental and Theoretical Study*, J. Phys. Chem. B **103**, 7627 (1999).
- 125.** F. Illas, G. Pacchioni, A. Pelmenschikov, L.G.M. Pettersson, C. Pisani, R. Dovesi, K.M. Neymann and N. Rösch, *Comment on First principles determination of the bonding mechanism and adsorption energy for CO/MgO(001) by L. Chen, R. Wu, N. Kioussis, and Q. Zhang, Chem. Phys. Lett. 290, 255-260 (1998)*, Chem. Phys. Letters **306**, 202 (1999).
- 126.** L. Triguero, O. Plashkevych, L.G.M. Pettersson and H. Ågren, *Separate state versus transition state Kohn-Sham calculations of X-ray photoelectron binding energies and chemical shifts*, J. El. Spec. **104**, 195 (1999).
- 127.** M. Nyberg, Y. Luo, L. Triguero, L.G.M. Pettersson and H. Ågren, *Core-hole effects in the X-ray absorption spectra of fullerenes*, Phys. Rev. B **60**, 7956 (1999).
- 128.** Y. Mochizuki, H. Ågren, L.G.M. Pettersson and V. Carravetta, *A theoretical investigation of sulphur K-shell X-ray absorption of cysteine*, Chem. Phys. Letters **309**, 241 (1999).

- 129.** M. Staufer, U. Birkenheuer, T. Belling, F. Nörtemann, N. Rösch, M. Stichler, D. Menzel, W. Wurth, L.G.M. Pettersson and A. Nilsson, *Interpretation of X-ray Emission Spectra: NO adsorbed on Ru(001)*, J. Chem. Phys. **111**, 4704 (1999).
- 130.** L.G.M. Pettersson, T. Hatsui, and N. Kosugi, *Ni 2p-3d photoabsorption and strong charge transfer satellites in divalent Ni complexes with molecular ligands. Evaluation of  $\pi$ -backdonation based on the DFT approach*, Chem. Phys. Letters, **311**, 299 (1999).
- 131.** L. Triguero, S. de Carolis, M. Baudin, M. Wójcik, K. Hermansson, M.A. Nygren and L.G.M. Pettersson, *Metal Oxides: O(2-) Chemistry and Dynamical Effects on Oxide Reactivity*, Faraday Discussion **114**, 351 (1999).
- 132.** A. Nilsson, J. Hasselström, A. Föhlisch, O. Karis, L.G.M. Pettersson, M. Nyberg and L. Triguero, *Probing Chemical Bonding in Adsorbates using X-ray Emission Spectroscopy*, J. Electron Spec. Rel. Phen. **110-111**, 15 (2000).
- 133.** A. Föhlisch, J. Hasselström, P. Bennich, N. Wassdahl, O. Karis, A. Nilsson, L. Triguero, M. Nyberg and L.G.M. Pettersson, *Ground-State Interpretation of X-Ray Emission Spectroscopy on Adsorbates: CO adsorbed on Cu(100)*, Phys. Rev. B **61**, 16229 (2000).
- 134.** J. Hasselström, O. Karis, M. Nyberg, L.G.M. Pettersson, M. Weinelt, N. Wassdahl and A. Nilsson, *The bonding and electronic structure changes upon adsorption of important functional groups: Glycine on copper*, J. Phys. Chem. B, **104**, 11480 (2000).
- 135.** O. Plashkevych, H. Ågren, L. Karlsson and L.G.M. Pettersson, *Calculations of valence electron binding energies using Kohn-Sham theory and transition potentials*, J. Electron Spec. Rel. Phen. **106**, 51 (2000).
- 136.** M. Nyberg, J. Hasselström, O. Karis, N. Wassdahl, M. Weinelt, A. Nilsson, L.G.M. Pettersson, *The electronic structure and surface chemistry of glycine adsorbed on Cu(110)*, J. Chem. Phys. **112**, 5420 (2000).
- 137.** L. Triguero, A. Föhlisch, P. Väterlein, J. Hasselström, M. Weinelt, L.G.M. Pettersson, Y. Luo, H. Ågren and A. Nilsson, *Direct Experimental Measurement of Donation/Backdonation in Unsaturated Hydrocarbon Bonding to Metals*, J. Am. Chem. Soc. **122**, 12310 (2000).
- 138.** A. Föhlisch, P. Bennich, J. Hasselström, O. Karis, A. Nilsson, M. Nyberg, L. Triguero and L.G.M. Pettersson, *The bonding of CO to Metal Surfaces*, J. Chem. Phys. **112**, 1946 (2000).
- 139.** O. Karis, J. Hasselström, N. Wassdahl, M. Weinelt, A. Nilsson, M. Nyberg, L.G.M. Pettersson, J. Stöhr and M.G. Samant, *The bonding of simple carboxylic acids on Cu(110)*, J. Chem. Phys. **112**, 8146 (2000).
- 140.** A. Föhlisch, M. Nyberg, J. Hasselström, O. Karis, L.G.M. Pettersson and A. Nilsson, *How CO adsorbs in different sites*, Phys. Rev. Letters **85**, 3309 (2000).
- 141.** A.G. Pelmenschikov, H. Strandh, L.G.M. Pettersson and J.R. Leszczynski, *Lattice Resistance to Dissolution of Si-O-Si Bonds of Silicate Minerals: Ab Initio Calculations of Cluster Models of  $\beta$ -Cristabolite Surfaces*, J. Phys. Chem. B, **104**, 5779 (2000).

142. A. Pelmenschikov, G. Morosi, A. Gamba, S. Coluccia, G. Martra and L.G.M. Pettersson, *Can the Three-coordinated Mg site of MgO Accommodate more than one CO Molecule?*, J. Phys. Chem. B, **104**, 11497 (2000).
143. Lars G.M. Pettersson, Anders Nilsson, Satish Myneni, Yi Luo, Mats Nyberg, Matteo Cavalleri, Lars Ojamäe, Lars-Åke Näslund, Hirohito Ogasawara, Michael Odelius and Alexander Pelmenschikov, *Electronic structure effects from hydrogen bonding in the liquid phase and in chemisorption: an integrated theory and experimental effort*, J. Synchrotron Rad. **8**, 136 (2001).
144. C. Kolczewski, R. Püttner, O. Plashkevych, H. Ågren, V. Staemmler, M. Martins, G. Snell, A.S. Schlachter, M. Sant'anna, G. Kaindl and L.G.M. Pettersson, *Detailed Study of pyridine at the C 1s and N 1s ionization thresholds: The influence of the vibrational fine structure*, J. Chem. Phys. **115**, 6426-6437 (2001).
145. A. Pelmenschikov, J. Leszczynski and L.G.M. Pettersson, *Mechanism of Dissolution of Neutral Silica Surfaces: Including Effect of Self-Healing*, J. Phys. Chem. A **105**, 9528-9532 (2001).
146. S. Myneni, Y. Luo, L.Å. Näslund, M. Cavalleri, L. Ojamäe, H. Ogasawara, A. Pelmenschikov, Ph. Wernet, P. Väterlein, C. Heske, Z. Hussain, L.G.M. Pettersson and A. Nilsson, *Spectroscopic probing of local hydrogen bonding structures in liquid water*, J Phys.: Condens. Mat. **14**, L213-L219 (2002) (Editor's Choice, Science, **295** (2002) 1975).
147. K.R. Wilson, M. Cavalleri, B.S. Rude, R.D. Schaller, A. Nilsson, L.G.M. Pettersson, N. Goldman, T. Catalano, J.D. Bozek, R.J. Saykally, *Characterization of hydrogen bond acceptor molecules at the water surface using near-edge x-ray absorption fine-structure spectroscopy and density functional theory*, J. Phys.: Condens. Mat. **14**, L221-L226 (2002) (Editor's Choice, Science, **295** (2002) 1975)
148. E.J. Karlsen and L.G.M. Pettersson,  *$N_2O$  decomposition over BaO: Including effects of coverage*, J. Phys. Chem. B, **106**, 5719-5721 (2002).
149. E.J. Karlsen, M.A. Nygren and L.G.M. Pettersson, *Theoretical study on the decomposition of  $N_2O$  over rocksalt metal-oxides: MgO-BaO*, J. Phys. Chem. A **106**, 7868-7875 (2002).
150. M. Cavalleri, H. Ogasawara, L. G. M. Pettersson and A. Nilsson, *The interpretation of X-ray absorption spectra in water and ice*, Chem. Phys. Letters **364**, 363-370 (2002).
151. U. Bergmann, Ph. Wernet, P. Glatzel, M. Cavalleri, L. G. M. Pettersson, M. Odelius, P.-C. Lin, A. Nilsson, and S. P. Cramer, *Oxygen K-edge Spectroscopy of Liquid Water and Ice: Implications on Local Structure Models*, Phys. Rev. B **66**, 092107 (2002).
152. H. Ogasawara, B. Brena, D. Nordlund, M. Nyberg, A. Pelmenschikov, L.G.M. Pettersson, and A. Nilsson, *Structure and Bonding of Water on Pt(111)*, Phys. Rev. Letters **89**, 276102 (2002); Physical Review Focus, December 31, 2002; Editor's Choice, Science **299**, 475 (2003); Highlight Angewandte Chemie **42**, 3458-3460 (2003).

- 153.** J.-L. Pascual and L.G.M. Pettersson, *Cluster Modelling of O(1s) Core Excitons at the (100) Surface of Alkaline Earth Oxides*, Mol. Phys. **101**, 255-265 (2003).
- 154.** S. Trasobares, C. Kolczewski, R. Räty, N. Borglund, A. Bassan, G. Hug, C. Colliex, S. Csillag and L.G.M. Pettersson, *Monitoring the Decomposition of Melamine in the Solid Phase by Electron Energy Loss Chronospectroscopy*, J. Phys. Chem. A **107**, 228-235 (2003).
- 155.** H. Öström, L. Triguero, K. Weiss, H. Ogasawara, M.G. Garnier, D. Nordlund, M. Nyberg, L.G.M. Pettersson and A. Nilsson, *Orbital rehybridization in n-octane adsorbed on Cu(110)*, J. Chem. Phys. **118**, 3782-3789 (2003).
- 156.** K. Weiss, H. Öström, L. Triguero, H. Ogasawara, M.G. Garnier, L.G.M. Pettersson and A. Nilsson, *XPS and XAS investigation of condensed and adsorbed n-octane on a Cu(110) surface*, J. El. Spec. Rel. Phen. **128**, 179-191 (2003).
- 157.** Elly J. Karlsen and Lars G.M. Pettersson, *Theoretical Study on the Decomposition Reactions of N<sub>2</sub>O with O<sup>-</sup>, O<sub>2</sub><sup>-</sup> and O<sub>3</sub><sup>-</sup>*, J. Phys. Chem. A **107**, 1641-1646 (2003).
- 158.** Elly J. Karlsen, Martin A. Nygren and Lars G.M. Pettersson, *Comparative Study on the Structures and Energetics of NO<sub>x</sub>, SO<sub>x</sub> and CO<sub>x</sub> on Alkaline-earth Metal Oxides*, J. Phys. Chem. B **107**, 7795-7802 (2003).
- 159.** H. Öström, L. Triguero, M. Nyberg, H. Ogasawara, L.G.M. Pettersson and A. Nilsson, *Bonding of saturated hydrocarbons to metal surfaces*, Phys. Rev. Letters **91**, 046102 (2003).
- 160.** Lars-Åke Näslund, Matteo Cavalleri, Hirohito Ogasawara, Anders Nilsson, Lars G.M. Pettersson, Philippe Wernet, David C. Edwards, Magnus Sandström, and Satish Myneni, *Direct evidence of orbital mixing between water and solvated transition metal ions: An oxygen 1s XAS and DFT study of aqueous systems*, J. Phys. Chem. A, **107**, 6869-6876 (2003).
- 161.** M. Nyberg, M. Odelius, A. Nilsson and L.G.M. Pettersson, *Hydrogen bonding between adsorbed glycine molecules on Cu(110)*, J. Chem. Phys. **119**, 12577-12585 (2003).
- 162.** Ph. Wernet, D. Nordlund, U. Bergmann, H. Ogasawara, M. Cavalleri, L. Å. Näslund, T. K. Hirsch, L. Ojamäe, P. Glatzel, M. Odelius, L.G.M. Pettersson, and A. Nilsson, *The structure of the first coordination shell in liquid water*, Science **304**, 995-999 (2004). Published on the web 1 April 2004; 10.1126/science.1096205. (Science Top Ten Breakthroughs 2004, Science **306**, 2013-2017 (2004)).
- 163.** H. Öström, A. Föhlisch, M. Nyberg, M. Weinelt, C. Heske, L.G.M. Pettersson and A. Nilsson, *Ethylene on Cu(110) and Ni(110): Electronic structure and bonding derived from X-ray spectroscopy and Theory*, Surf. Sci. **559**, 85-99 (2004).
- 164.** D. Nordlund, H. Ogasawara, Ph. Wernet, M. Nyberg, M. Odelius, L.G.M. Pettersson, and A. Nilsson, *Surface structure of thin ice films*, Chem. Phys. Letters **395**, 161-165 (2004).
- 165.** A. Nilsson and L.G.M. Pettersson, *Chemical Bonding on Surfaces Probed by X-ray Emission Spectroscopy and Density Functional Theory*, Surf. Sci. Rep. **55**, 49-167 (2004).

- 166.** H. Öström, D. Nordlund, H. Ogasawara, K. Weiss, L. Triguero, L.G.M. Pettersson and A. Nilsson, *Geometric structure and chemical bonding of acetylene adsorbed on Cu(110)*, Surf. Sci. **565** (2-3), 206-222 (2004).
- 167.** K. Andersson, M. Nyberg, H. Ogasawara, D. Nordlund, T. Kendlewicz, C.S. Doyle, G.E. Brown, Jr, L.G.M. Pettersson and A. Nilsson, *Experimental and Theoretical Characterization of the Structure of Defects at the Pyrite FeS<sub>2</sub>(100) Surface*, Phys. Rev. B **70**, 195404 (2004).
- 168.** M. Cavalleri, M. Odelius, A. Nilsson and L.G.M. Pettersson, *X-ray Absorption Spectra within a plane-wave Car-Parrinello Molecular Dynamics Framework*, J. Chem. Phys. **121**, 10065-10075 (2004).
- 169.** B. Brena, D. Nordlund, M. Odelius, H. Ogasawara, A. Nilsson and L.G.M. Pettersson, *Ultrafast Molecular Dissociation of Water in Ice*, Phys. Rev. Letters **93**(14) 148302 (2004).
- 170.** M. Hakala, S. Huotari, K. Hämäläinen, Ph. Wernet, A. Nilsson, S. Manninen and L.G.M. Pettersson, *Compton profiles for water and mixed water-neon clusters: measure of coordination*, Phys. Rev. B **70**, 125413 (2004).
- 171.** O. Takahashi and L.G.M. Pettersson, *Functional Dependence of Core-Excitation Energies*, J. Chem. Phys. **121**, 10339-10345 (2004).
- 172.** K. Andersson, A. Nikitin, L.G.M. Pettersson, A. Nilsson and H. Ogasawara, *Water dissociation on Ru(001): An activated process*, Phys. Rev. Letters **93**, 196101 (2004).
- 173.** E. Damian, A. Molla-Abbassi, F. Jalilehvand, L.G.M. Pettersson and M. Sandström, *Sulfur K-Edge X-Ray Absorption Spectra for Dimethyl Sulfoxide in the Solvated Thallium(III), Indium(III), Gallium(III) and Aluminum(III) Ions*, Phys. Scripta **T115**, 1077-1079 (2005).
- 174.** O. Takahashi, M. Joyabu, M. Mitani, K. Saito, Y. Senba, H. Yoshida, A. Hiraya and L.G.M. Pettersson, *Studies of the X-ray Absorption Spectra of Some Methylcyano Esters*, J. El. Spec. Rel. Phen. **142**, 113-119 (2005).
- 175.** K.R. Wilson, M. Cavalleri, B.S. Rude, R.D. Schaller, T. Catalano, A. Nilsson, R.J. Saykally, and L.G.M. Pettersson, *X-ray Absorption Spectroscopy of Liquid Methanol Microjets: Bulk Electronic Structure and Hydrogen Bonding Network*, J. Phys. Chem. B **109**(20), 10194 – 10203 (2005).
- 176.** A. Nilsson, L. G. M. Pettersson, B. Hammer, T. Bligaard, C. H. Christensen and J. K. Nørskov, *The Electronic Structure Effect in Heterogeneous Catalysis*, Catal. Letters **100**, 111 (2005).
- 177.** A. Nilsson, H. Ogasawara, M. Cavalleri, D. Nordlund, M. Nyberg, Ph. Wernet and L. G. M. Pettersson, *The Hydrogen Bond in Ice Probed by Soft X-ray Spectroscopy and Density Functional Theory*, J. Chem. Phys. **122**, 154505 (2005).
- 178.** A. Nilsson, Ph. Wernet, D. Nordlund, U. Bergmann, M. Cavalleri, M. Odelius, H. Ogasawara, L.-Å. Näslund, T. K. Hirsch, L. Ojamäe, P. Glatzel and L. G. M. Pettersson, *Comment on “Energetics of Hydrogen Bond Network Rearrangements in Liquid Water”*, Science **308**, 793a (2005).

- 179.** K. Andersson, A. Gómez, C. Glover, D. Nordlund, H. Öström, T. Schiros, O. Takahashi, H. Ogasawara, L.G.M Pettersson and A. Nilsson, *Molecularly Intact and Dissociative Adsorption of Water on Clean Cu(110): A Comparison with the Water/Ru(001) system*, Surf. Sci. Letters **585**, L183-L189 (2005).
- 180.** Lars-Åke Näslund, David C. Edwards, Uwe Bergmann, Philippe Wernet, Hirohito Ogasawara, L.G.M Pettersson, Satish Myneni and Anders Nilsson, *X-ray Absorption Spectroscopy study of the hydrogen bond network in the bulk water of aqueous solutions*, J. Phys. Chem. A **109**, 5995-6002 (2005).
- 181.** M. Odelius, H. Ogasawara, D. Nordlund, O. Fuchs, L. Weinhardt, F. Maier, E. Umbach, C. Heske, Y. Zubavicus, M. Grunze, J. Denlinger, L.G.M. Pettersson and A. Nilsson, *Ultrafast core-hole induced dynamics in water probed by x-ray emission spectroscopy*, Phys. Rev. Letters **94**, 227401 (2005).
- 182.** L.Å. Näslund, J. Lüning, Y. Ufuktepe, H. Ogasawara, Ph. Wernet, U. Bergmann, L. G. M. Pettersson and A. Nilsson, *X-ray absorption spectroscopy measurements of liquid water*, J. Phys. Chem. B **109**, 13835-13839 (2005).
- 183.** Morten B. Jensen, Lars G. M. Pettersson, Ole Swang, and Unni Olsbye, *CO<sub>2</sub> Sorption on Different Sites on MgO and CaO Surfaces: A Comparative Quantum Chemical Cluster Study*, J. Phys. Chem. B **109**, 16774 (2005).
- 184.** M. Cavalleri, D. Nordlund, M. Odelius, A. Nilsson, and L.G.M. Pettersson, *Half or full core-hole in Density Functional Theory X-ray absorption spectrum calculations of water?*, Phys. Chem. Chem. Phys. **7**, 2854 – 2858 (2005).
- 185.** Ph. Wernet, D. Testemale, J.-L. Hazemann, R. Argoud, P. Glatzel, L.G.M. Pettersson, A. Nilsson and U. Bergmann, *Spectroscopic characterization of microscopic hydrogen bonding disparities in supercritical water*, J. Chem. Phys. **123**, 154503 (2005).
- 186.** M. Nyberg, L. Triguero, A. Bassan, L.G.M. Pettersson, A. Föhlisch, and A. Nilsson, *Bonding in Metal-Carbonyls: A Comparison with Experiment and Calculations on Adsorbed CO*, J. Mol. Struc. (THEOCHEM) **762**, 123-132 (2006).
- 187.** M. Odelius, M. Cavalleri, A. Nilsson and L.G.M. Pettersson, *The X-ray Absorption Spectrum of Liquid Water from Molecular Dynamics Simulations: Asymmetric Model*, Phys. Rev. B. **73**, 024205 (2006).
- 188.** Osamu Takahashi, Michael Odelius, Dennis Nordlund, Anders Nilsson, and Lars G. M. Pettersson, *Auger Decay Calculations with Core-hole Excited State Molecular Dynamics Simulations of Water*, J. Chem. Phys. **124**, 064307 (2006).
- 189.** M. Hakala, K. Nygård, S. Manninen, L.G.M. Pettersson, K. Hämäläinen, *Intra- and intermolecular effects in the Compton profile of water*, Phys. Rev. B **73**, 035432 (2006).
- 190.** O. Takahashi, K. Tabayashi, Shin-ichi Wada, R. Sumii, K. Tanaka, M. Odelius, and L. G. M. Pettersson, *Theoretical Study of ion desorption from PMMA and PiPAc thin films*, J. Chem. Phys. **124**, 124901 (2006).

- 191.** E. Melero García, A. Kivimäki, J. Álvarez Ruiz, M. Coreno, M. de Simone, L.G.M. Pettersson, K.C. Prince, and R. Richter, *Fluorescence emission of excited hydrogen atoms after core excitation of water vapor*, Phys. Rev. Letters **96**, 063003 (2006).
- 192.** H. Öström, H. Ogasawara, L.-Å Näslund, L.G.M. Pettersson and A. Nilsson, *Physisorption-induced C-H bond elongation in methane*, Phys. Rev. Letters **96**, 146104 (2006).
- 193.** Matteo Cavalleri, Lars-Åke Näslund, David C. Edwards, Philippe Wernet, Hirohito Ogasawara, Satish Myneni, Lars Ojamäe, Michael Odelius, Anders Nilsson, and Lars G.M. Pettersson, *The local structure of protonated water from X-ray absorption and Density Functional Theory*, J. Chem. Phys. **124**, 194508 (2006)
- 194.** Gordon E. Brown, Jr., Anders Nilsson, Alfred M. Spormann, William P. Addiego, Karim Benzerara, Uwe Bergmann, Hendrik Bluhm, Bryan A. Brown, Georges Calas, Anne M. Chaka, Brent R. Constantz, Francois Farges, Scott E. Fendorf, Andrea L. Foster, Farid Juillot, Guillaume Morin, Satish C.B. Myneni, Lars G.M. Pettersson, Kevin M. Rosso, James J. Rytuba, Miquel Salmerón, Jennifer Saltzman, Michael Toney, Thomas P. Trainor, and Tae-Hyun Yoon, *The Stanford Environmental Molecular Science Institute – A Focus on Chemical and Microbial Processes at Environmental Interfaces*, The Geochemical News **128**, 7 (2006).
- 195.** M. Hakala, K. Nygård, S. Manninen, S. Huotari, T. Buslaps, A. Nilsson, L.G.M. Pettersson and K. Hääläinen, *Correlation of hydrogen bond lengths and angles in liquid water based on Compton scattering*, J. Chem. Phys. **125**, 084504 (2006).
- 196.** T. Schiros, H. Ogasawara, O. Takahashi, H. Öström, K. Andersson, L.G.M. Pettersson, A. Nilsson, S. Haq, and A. Hodgson, *Structure of water adsorbed on Cu(110): H-up, H-down, or both?*, Chem. Phys. Letters **429**, 415 (2006).
- 197.** K. Nygård, M. Hakala, S. Manninen, A. Andrejczuk, M. Itou, Y. Sakurai, L.G.M. Pettersson, and K. Hääläinen, *Compton scattering study of water versus ice Ih: intra- and intermolecular structure*, Phys. Rev. E **74**, 031503 (2006).
- 198.** M. Leetmaa, M. Ljungberg, H. Ogasawara, M. Odelius, L.-Å. Näslund, A. Nilsson and L.G.M. Pettersson, *Are Recent Water Models Obtained by Fitting Diffraction Data Consistent with IR/Raman and X-ray Absorption Spectra?*, J. Chem. Phys. **125**, 244510 (2006).
- 199.** Susumu Yamamoto, Klas Andersson, Hendrik Bluhm, Guido Ketteler, David E. Starr, Theanne Schiros, Hirohito Ogasawara, Lars G. M. Pettersson, Miquel Salmerón, and Anders Nilsson, *Hydroxyl Induced Wetting of Metals by Water at Near Ambient Conditions*, J. Phys. Chem. C **111**, 7848 (2007).
- 200.** U. Bergmann, D. Nordlund, Ph. Wernet, M. Odelius, L. G. M. Pettersson, A. Nilsson, *Isotope Effects in Liquid Water probed by X-ray Raman Spectroscopy*, Phys. Rev. B **76**, 024202 (2007).
- 201.** Emiliana Damian Risberg, Lars Eriksson, János Mink, Lars G. M. Pettersson, Mikhail Yu. Skripkin and Magnus Sandström, *Sulfur X-ray absorption and vibrational spectroscopic study of sulfite, sulfur dioxide and sulfonate solutions and the substituted sulfonate ions  $X_3CSO_3^-$  ( $X=H, Cl, F$ )*, Inorg. Chem. **46**, 8332-8348 (2007).

- 202.** Klas Andersson, Guido Ketteler, Hendrik Bluhm, Susumu Yamamoto, Hirohito Ogasawara, Lars G. M. Pettersson, Miquel Salmerón, Anders Nilsson, *Bridging the Pressure Gap in Water and Hydroxyl Chemistry on Metal Surfaces: the Cu(110) case*, J. Phys. Chem. C **111**, 14493-14499 (2007).
- 203.** T. Schiros, L.-Å. Näslund, K. Andersson, J. Gyllenpalm, G.S. Karlberg, M. Odelius, H. Ogasawara, L.G.M. Pettersson and A. Nilsson, *Structure and bonding of water-hydroxyl mixed phase on Pt(111)*, J. Phys. Chem. C **111**, 15003-15012 (2007).
- 204.** H. Öström, H. Ogasawara, L.-Å. Näslund, K. Andersson, L.G.M. Pettersson and A. Nilsson, *Geometric and electronic structure of methane adsorbed on a Pt surface*, J. Chem. Phys. **127**, 144702 (2007).
- 205.** D. Nordlund, H. Ogasawara, H. Bluhm, O. Takahashi, M. Odelius, M. Nagasano, L.G.M. Pettersson, and A. Nilsson, *Probing the Electron Delocalization in Liquid Water and Ice at Attosecond Time Scales*, Phys. Rev. Letters **99**, 217406 (2007).
- 206.** Anders Nilsson and Lars G.M. Pettersson, *Adsorbate Electronic Structure and Bonding on Metal Surfaces*, in *Chemical Bonding at Surfaces and Interfaces*, A. Nilsson, L.G.M. Pettersson and J.K. Nørskov, Eds. (Elsevier, Amsterdam, 2008). p57-142.
- 207.** Anders Nilsson, Lars G.M. Pettersson, and Jens K. Nørskov, *Chemical Bonding at Surfaces and Interfaces Preface*, in *Chemical Bonding at Surfaces and Interfaces*, A. Nilsson, L.G.M. Pettersson and J.K. Nørskov, Eds. (Elsevier, Amsterdam, 2008), pages XI-XII.
- 208.** Klas Andersson, Guido Ketteler, Hendrik Bluhm, Susumu Yamamoto, Hirohito Ogasawara, Lars G. M. Pettersson, Miquel Salmerón, and Anders Nilsson, *Auto-catalytic water dissociation on Cu(110) at near ambient conditions*, J. Am. Chem. Soc. **130**, 2793 (2008).
- 209.** I. Waluyo, D. Nordlund, L.-Å. Näslund, H. Ogasawara, L.G.M. Pettersson, A. Nilsson, *Spectroscopic evidence for the formation of 3-D crystallites during isothermal heating of amorphous ice on Pt(111)*, Surface Science **602**, 2004 (2008).
- 210.** Takashi Tokushima, Yoshihisa Harada, Osamu Takahashi, Yasunori Senba, Haruhiko Ohashi, Lars G.M. Pettersson, Anders Nilsson, and Shik Shin, *High Resolution X-ray Emission Spectroscopy of Liquid Water: The Observation of Two Structural Motifs*, Chem. Phys. Letters **460**, 387-400 (2008); FRONTIERS paper (cover)  
<http://dx.doi.org/10.1016/j.cplett.2008.04.077>.
- 211.** D. Nordlund, M. Odelius, H. Bluhm, H. Ogasawara, L.G.M. Pettersson, and A. Nilsson, *Electronic structure effects in liquid water studied by photoelectron spectroscopy and density functional theory*, Chem. Phys. Letters **460**, 86-92 (2008).
- 212.** L. G. M. Pettersson, T. Tokushima, Y. Harada, O. Takahashi, S. Shin and A. Nilsson, *Comment on “Isotope and Temperature Effects in Liquid Water Probed by X-ray Absorption and Resonant X-ray Emission Spectroscopy”*, Phys. Rev. Letters **100**, 249801 (2008).

- 213.** Mikael Leetmaa, Kjartan Thor Wikfeldt, Mathias P. Ljungberg, Michael Odelius, Jan Swenson, Anders Nilsson, and Lars G.M. Pettersson, *Diffraction and IR/Raman Data do not Prove Tetrahedral Water*, J. Chem. Phys. **129**, 084502 (2008).
- 214.** M. Tatarkhanov, E. Fomin, M. Salmerón, K. Andersson, H. Ogasawara, L.G.M. Pettersson, A. Nilsson, J.I. Cerdá, *The structure of mixed H<sub>2</sub>O/OH monolayer films on Ru(0001)*, J. Chem. Phys. **129**, 154109 (2008).
- 215.** A. Mijovilovich, L.G.M. Pettersson, S. Mangold, M. Janousch, J. Susini, M. Salome, F.M.F. de Groot and B.M. Weckhuysen, *The Interpretation of Sulfur K-edge XANES spectra: A case Study on Thiophene and Aliphatic Sulfur Compounds*, J. Phys. Chem. A **113**, 2750-2756 (2009).
- 216.** Mikael Leetmaa, Mathias Ljungberg, Anders Nilsson, and Lars G.M. Pettersson, *X-ray Spectroscopy Calculations within Kohn-Sham DFT: Theory and Applications*, in *Computational methods in Catalysis and Materials Science*, p. 221-264, Ed. R.A. van Santen, P. Sautet (Wiley-VCH, 2009).
- 217.** E. Damian-Risberg, F. Jalilehvand, B. Leung, L.G.M. Pettersson and M. Sandström, *Theoretical and experimental sulfur K-edge X-ray absorption spectroscopic (XANES) study of cysteine, methionine, methionine sulfoxide and cystine*, Dalton Transactions 3542-3558 (2009).
- 218.** Kjartan T. Wikfeldt, Mikael Leetmaa, Mathias P. Ljungberg, Anders Nilsson, and Lars G.M. Pettersson, *On the Range of Water Structure Models Compatible with X-ray and Neutron Diffraction Data*, J. Phys. Chem. B **113**, 6246-6255 (2009).
- 219.** Mathias P. Ljungberg, A. P. Lyubartsev, Anders Nilsson, and Lars G.M. Pettersson, *Assessing the E-field approximation to IR and Raman Spectra of Dilute HOD in D<sub>2</sub>O*, J. Chem. Phys. **131**, 034501 (2009).
- 220.** R. Alonso Mori, E. Paris, G. Giuli, S. Eeckhout, M. Kavcic, M. Zitnic, K. Bucar, L.G.M. Pettersson, and P. Glatzel, *The electronic structure of Sulfur studied by X-ray absorption and emission spectroscopy*, Analytical Chemistry **81**, 6516-6525 (2009).
- 221.** Iradwikanari Waluyo, Dennis Nordlund, Uwe Bergmann, Lars G.M. Pettersson, and Anders Nilsson, *Increased Fraction of Weakened Hydrogen Bonds of Water in AOT Reverse Micelles*, J. Chem. Phys. **131**, 031103 (2009).
- 222.** Congcong Huang, K. T. Wikfeldt, T. Tokushima, D. Nordlund, Y. Harada, U. Bergmann, M. Niebuhr, T. M. Weiss, Y. Horikawa, M. Leetmaa, M. P. Ljungberg, O. Takahashi, A. Lenz, L. Ojamäe, A. P. Lyubartsev, S. Shin, L. G. M. Pettersson and A. Nilsson, *The Inhomogeneous Structure of Water at Ambient Conditions*, Proc. Natl. Acad. Sci. (USA) **106**, 15214–15218 (2009).
- 223.** D. Nordlund, H. Ogasawara, K.J. Andersson, M. Tatarkhanov, M. Salmerón, L. G. M. Pettersson and A. Nilsson, *Sensitivity of X-ray Absorption Spectroscopy to Hydrogen Bond Topology*, Phys. Rev. B **80**, 233404 (2009).
- 224.** A. Nilsson and L.G.M. Pettersson, *Chemical Bonding on Metal Surfaces; Synergy between Theory and Experiment*, pages 253-274, in *Model Systems in Catalysis: From Single Crystals*

*and Size-Selected Clusters to Supported Enzyme Mimics*, edited by R.M. Rioux (Springer Science+Business Media, 2010).

- 225.** Mikael Leetmaa, Kjartan Thor Wikfeldt, and Lars G.M. Pettersson, *SpecSwap-RMC: A novel reverse Monte Carlo approach using a discrete set of local configurations and pre-computed properties*, J. Phys.: Cond. Mat. **22**, 135001 (2010).
- 226.** T. Schiros, O. Takahashi, K.J. Andersson, H. Öström, L.G.M. Pettersson, A. Nilsson and H. Ogasawara, *The Role of Substrate Electrons in the Wetting of a Metal Surface*, J. Chem. Phys. **132**, 094701 (2010).
- 227.** C. Huang, K. T. Wikfeldt, T. Tokushima, D. Nordlund, Y. Harada, U. Bergmann, M. Niebuhr, T. M. Weiss, Y. Horikawa, M. Leetmaa, M. P. Ljungberg, O. Takahashi, A. Lenz, L. Ojamäe, A. P. Lyubartsev, S. Shin, L. G. M. Pettersson and A. Nilsson, *Reply to Soper "Fluctuations in water around a bimodal distribution of local hydrogen bonded structural motifs"*, Proc. Natl. Acad. Sci. (USA) **107**, E45 (2010).
- 228.** Kjartan Thor Wikfeldt, Mikael Leetmaa, Amber Mace, Anders Nilsson, and Lars G.M. Pettersson, *Oxygen-oxygen correlations in liquid water; addressing the discrepancy between diffraction and EXAFS using a novel multiple -data set fitting technique*, J. Chem. Phys. **132**, 104513 (2010).
- 229.** M. Leetmaa, M. P. Ljungberg, A. Lyubartsev, A. Nilsson, and L. G. M. Pettersson, *Theoretical Approximations to X-ray Absorption Spectroscopy of Liquid Water and Ice*, J. Electron Spec. Rel. Phen. **177**, 135-157 (2010).
- 230.** A. Nilsson, D. Nordlund, I. Waluyo, N. Huang, H. Ogasawara, S. Kaya, U. Bergmann, L.-Å. Näslund, H. Öström, Ph. Wernet, K. Andersson, T. Schiros and L. G. M. Pettersson, *X-ray Absorption Spectroscopy and X-ray Raman Scattering of Water; An Experimental View*, J. Electron Spec. Rel. Phen. **177**, 99-129 (2010).
- 231.** Takashi Tokushima, Yoshihisa Harada, Yuka Horikawa, Osamu Takahashi, Yasunori Senba, Haruhiko Ohashi, Lars G.M. Pettersson, Anders Nilsson, and Shik Shin, *High resolution X-ray emission spectroscopy of water and its assignment based on two structural motifs*, J. Electron Spec. Rel. Phen. **177**, 192-205 (2010).
- 232.** T. Schiros, K.J. Andersson, L.G.M. Pettersson, A. Nilsson, and H. Ogasawara, *Chemical bonding of water to metal surfaces studied with core-level spectroscopies*, J. Electron Spec. Rel. Phen. **177**, 85–98 (2010).
- 233.** T. Schiros, H. Ogasawara, K. Andersson, J. Ren, Sh. Meng, G. Karlberg, L.-Å. Näslund, M. Odelius, A. Nilsson, and L.G.M. Pettersson, *Cooperativity in surface- and hydrogen-bonding of water and hydroxyl at metal surfaces*, J. Phys. Chem. C **114**, 10240–10248 (2010).
- 234.** T. Anniyev, H. Ogasawara, M.P. Ljungberg, K. T. Wikfeldt, J. B. MacNaughton, L.-Å. Näslund, U. Bergmann, S. Koh, P. Strasser, L.G.M. Pettersson and A. Nilsson, *Complementarity between high-energy photoelectron and L-edge spectroscopy for probing the electronic structure of 5d transition metal catalysts*, Phys. Chem. Chem. Phys. **12**, 5694-5700 (2010).

- 235.** R. Alonso Mori, E. Paris, G. Giuli, S.G. Eeckhout, M. Kavčič, M. Žitnik, K. Bučar, L.G.M. Pettersson, P. Glatzel, *Sulfur-Metal Orbital Hybridization in Sulfur-Bearing Compounds Studied by X-ray Emission Spectroscopy*, Inorganic Chemistry **49**, 6468 (2010).
- 236.** A. Mijovilovich, L.G.M. Pettersson, F.M.F. de Groot and B.M. Weckhuysen, *Functional groups and sulfur K-edge XANES spectra: Study of sulfides and disulfides*, J. Phys. Chem. A **114**, 9523-9528 (2010).
- 237.** Congcong Huang, T. M. Weiss, D. Nordlund, K. T. Wikfeldt, L. G. M. Pettersson and A. Nilsson, *Increasing correlation length in bulk supercooled H<sub>2</sub>O, D<sub>2</sub>O and NaCl solution determined from small angle x-ray scattering*, J. Chem. Phys. **133**, 134504 (2010).
- 238.** D. J. Miller, H. Öberg, L.-Å. Näslund, T. Anniyev, H. Ogasawara, L. G. M. Pettersson and A. Nilsson, *Low O<sub>2</sub> Dissociation Barrier on Pt(111) due to Adsorbate-Adsorbate Interactions*, J. Chem. Phys. **133**, 224701 (2010).
- 239.** M. P. Ljungberg, A. Nilsson, and L. G. M. Pettersson, *Semiclassical description of nuclear dynamics in x-ray emission of water*, Phys. Rev. B **82**, 245115 (2010).
- 240.** Daniel Friebel, Daniel J. Miller, Christopher P. O'Grady, Toyli Anniyev, John Bargar, Uwe Bergmann, Hirohito Ogasawara, Kjartan Thor Wikfeldt, Lars G. M. Pettersson, Anders Nilsson, *In situ x-ray probing reveals fingerprints of surface platinum oxide*, Phys. Chem. Chem. Phys. **13**, 262-266 (2011).
- 241.** M. P. Ljungberg, L. G. M. Pettersson, and A. Nilsson, *Vibrational interference effects in x-ray emission of a model water dimer: implications for the interpretation of the liquid spectrum*, J. Chem. Phys. **134**, 044513 (2011).
- 242.** Iradwikanari Waluyo, Congcong Huang, Dennis Nordlund, Uwe Bergmann, Thomas M. Weiss, Lars G.M. Pettersson, and Anders Nilsson, *The structure of water in the hydration shell of cations from x-ray Raman and small angle x-ray scattering measurements*, J. Chem. Phys. **134**, 064513 (2011).
- 243.** K. T. Wikfeldt, C. Huang, A. Nilsson and L. G. M. Pettersson, *Enhanced small-angle scattering connected to the Widom line in simulations of supercooled water*, J. Chem. Phys. **134**, 214506 (2011).
- 244.** Iradwikanari Waluyo, Congcong Huang, Dennis Nordlund, Thomas M. Weiss, Lars G.M. Pettersson, and Anders Nilsson, *Increased fraction of low-density structures in aqueous solutions of fluoride*, J. Chem. Phys. **134**, 224507 (2011).
- 245.** M. P. Ljungberg, J. J. Mortensen, and L. G. M. Pettersson, *An implementation of core level spectroscopies in a real space Projector Augmented Wave density functional theory code*, J. Electron Spec. Rel. Phen. **184**, 427– 439 (2011).
- 246.** Andreas Møgelhøj, André Kelkkanen, K. Thor Wikfeldt, Jakob Schiøtz, Jens Jørgen Mortensen, Lars G.M. Pettersson, Bengt I. Lundqvist, Karsten W. Jacobsen, Anders Nilsson and Jens K. Nørskov, *Ab initio van der Waals interactions in simulations of water alter structure from mainly tetrahedral to high-density-like*, J. Phys. Chem. B **115**, 14149–14160 (2011); doi:10.1021/jp2040345

- 247.** A. Nilsson and L. G. M. Pettersson, *Perspective on the Structure of Liquid Water*, Chem. Phys. **389**, 1-34 (2011).
- 248.** Jianping Xiao, Agnieszka Kuc, Suman Pokhrel, Marco Schowalter, Satyan Porlapalli, Andreas Rosenauer, Thomas Frauenheim, Lutz Mädler, Lars G.M. Pettersson, Thomas Heine, *Evidence for  $Fe^{2+}$  in Wurtzite coordination: iron doping stabilizes ZnO nanoparticles*, SMALL, **7**, 2879–2886 (2011).
- 249.** K. T. Wikfeldt, A. Nilsson and L. G. M. Pettersson, *Spatially Inhomogeneous Bimodal Inherent Structure in Simulated Liquid Water*, Phys. Chem. Chem. Phys. **13**, 19918-19924 (2011). doi:10.1039/c1cp22076d, [arXiv:1106.5038v1](https://arxiv.org/abs/1106.5038v1).
- 250.** N. Huang, D. Nordlund, C. Huang, U. Bergmann, T. M. Weiss, L. G. M. Pettersson, A. Nilsson, *X-ray Raman scattering provides evidence for interfacial acetonitrile-water dipole interactions in aqueous solutions*, J. Chem. Phys. **135**, 164509 (2011); doi:10.1063/1.3655468.
- 251.** D. J. Miller, H. Öberg, S. Kaya, D. Friebel, H. Bluhm, T. Anniyev, H. Ogasawara, H. Sanchez Casalongue, L. G. M. Pettersson and A. Nilsson, *Oxidation of Pt(111) under near-ambient conditions*, Phys. Rev. Letters **107**, 195502 (2011).
- 252.** Congcong Huang, K. T. Wikfeldt, D. Nordlund, U. Bergmann, T. McQueen, J. Sellberg, L. G. M. Pettersson and A. Nilsson, *Wide-Angle X-ray Diffraction and Molecular Dynamics Study of Medium-range Order in Ambient and Hot Water*, Phys. Chem. Chem. Phys. **13**, 19997-20007 (2011). doi:10.1039/c1cp22804h, <http://arxiv.org/abs/1107.4795>
- 253.** K.T. Wikfeldt, L.G.M. Pettersson, and A. Nilsson, *Liquid Water Structure from X-ray Spectroscopy and Simulations*, International School of Physics "Enrico Fermi", Course CLXXVI - "Complex materials in physics and biology" (IOS Press, Amsterdam, 2012).
- 254.** J. Gladh, H. Öberg, Jibiao Li, M. P. Ljungberg, A. Matsuda, H. Ogasawara, A. Nilsson, L. G. M. Pettersson, and H. Öström, *X-ray Emission Spectroscopy and Density Functional Study of CO/Fe(100)*, J. Chem. Phys. **136**, 034702 (2012).
- 255.** Takashi Tokushima, Yuka Horikawa, Hidemi Arai, Yoshihisa Harada, Osamu Takahashi, Lars G.M. Pettersson, Anders Nilsson, and Shik Shin, *Polarization dependent resonant x-ray emission spectroscopy of  $D_2O$  and  $H_2O$  water; assignment of the local molecular orbital symmetry*, J. Chem. Phys., **136**, 044517 (2012).
- 256.** Ningdong Huang, Daniel Schlesinger, Dennis Nordlund, Congcong Huang, Tolek Tyliszczak, Thomas M. Weiss, Yves Acremann, Lars G. M. Pettersson, Anders Nilsson, *Microscopic Probing of the Size Dependence in Hydrophobic Solvation*, J. Chem. Phys. **136**, 074507 (2012).
- 257.** H. Öberg, Y. Nestsiarenka, A. Matsuda, J. Gladh, T. Hansson, L. G. M. Pettersson and H. Öström, *Adsorption and cyclotrimerization kinetics of  $C_2H_2$  at a Cu(110) surface*, J. Phys. Chem. C **116**, 9550-9560 (2012); <http://dx.doi.org/10.1021/jp300514f>.
- 258.** Anders Nilsson, Congcong Huang and Lars G.M. Pettersson, *Fluctuations in Ambient Water*, J. Mol. Liq. **176**, 2-16 (2012); doi:10.1016/j.molliq.2012.06.021.

259. Theanne Schiros, Dennis Nordlund, Lucia Pálová, Deborah Prezzi, Liuyan Zhao, Keun Soo Kim, Ulrich Wurstbauer, Christopher Gutiérrez, Dean Delongchamp, Cherno Jaye, Daniel Fischer, Hirohito Ogasawara, Lars G.M. Pettersson, David R. Reichman, Philip Kim, Mark S. Hybertsen, Abhay N. Pasupathy, *Connecting dopant bond type with electronic structure in N-doped graphene*, Nano Letters, **12**, 4025–4031 (2012).
260. Anders Nilsson, Takashi Tokushima, Yuka Horikawa, Yoshihisa Harada, Mathias P. Ljungberg, Shik Shin, and Lars G.M. Pettersson, *Resonant Inelastic X-Ray Scattering of Liquid Water*, J. El. Struc. Rel. Phenom. **188**, 84–100 (2013); doi:10.1016/j.elspec.2012.09.011.
261. Sarp Kaya, Daniel Schlesinger, Susumu Yamamoto, John T. Newberg, Hendrik Bluhm, Hirohito Ogasawara, Tom Kendelewicz, Gordon E. Brown Jr., Lars G. M. Pettersson and Anders Nilsson, *Highly Compressed Two-Dimensional Form of Water at Ambient Conditions*, Sci. Rep. **3**, 1074 (2013). doi:10.1038/srep01074
262. M. Dell'Angela, T. Anniyev, M. Beye, R. Coffee, A. Föhlisch, J. Gladh, T. Katayama, S. Kaya, O. Krupin, A. Møgelhøj, D. Nordlund, J. K. Nørskov, H. Öberg, H. Ogasawara, H. Öström, L. G. M. Pettersson, W. F. Schlotter, J. A. Sellberg, F. Sorgenfrei, J. Turner, M. Wolf, W. Wurth, A. Nilsson, *Real-Time Observation of Surface Bond Breaking with an X-ray Laser*, Science **339**, 1302-1305 (2013); doi:10.1126/science.1231711 (March 15, 2013).
263. Lawrie B. Skinner, Congcong Huang, Daniel Schlesinger, Lars G.M. Pettersson, Anders Nilsson, Chris J. Benmore, *Benchmark oxygen-oxygen pair-distribution function of ambient water from x-ray diffraction measurements with a wide Q-range*, J. Chem. Phys. **138**, 074506 (2013); doi: 10.1063/1.4790861.
264. Chen Chen, Congcong Huang, Iradwikanari Waluyo, Dennis Nordlund, Tsu-Chien Weng, Dimosthenis Sokaras, Thomas Weiss, Uwe Bergmann, Lars G.M. Pettersson and Anders Nilsson, *Solvation Structures of Protons and Hydroxide Ions in Water*, J. Chem. Phys. **138**, 154506 (2013).
265. M. Beye, T. Anniyev, R. Coffee, M. Dell'Angela, A. Föhlisch, J. Gladh, T. Katayama, S. Kaya, O. Krupin, A. Møgelhøj, A. Nilsson, D. Nordlund, J. K. Nørskov, H. Öberg, H. Ogasawara, L.G.M. Pettersson, W. F. Schlotter, J. A. Sellberg, F. Sorgenfrei, J. J. Turner, M. Wolf, W. Wurth and H. Öström, *Selective ultrafast probing of transient hot chemisorbed and precursor states of CO on Ru(0001)*, Phys. Rev. Letters **110**, 186101 (2013).
266. Pradeep Kumar, K. Thor Wikfeldt, Daniel Schlesinger, Lars G.M. Pettersson and H. Eugene Stanley, *The Boson peak in supercooled water*, (Nature) Scientific Reports **3**, 1980 (2013) DOI: 10.1038/srep01980.
267. Lars G.M. Pettersson, *News and Views: Radical water*, Nature Chem. **5**, 553-554 (2013).
268. T. Schiros, K.J. Andersson, J. MacNaughton, J. Gladh, A. Matsuda, H. Öström, O. Takahashi, L.G.M. Pettersson, A. Nilsson, and H. Ogasawara, *Unique Water-Water Coordination Tailored by a Metal Surface*, J. Chem. Phys. **138**, 234708 (2013).
269. Henrik Öberg, Toyli Anniyev, Aleksandra Vojvodic, Sarp Kaya, Hirohito Ogasawara, Daniel Friebel, Daniel J. Miller, Dennis Nordlund, Mathias P. Ljungberg, Frank Abild-

- Pedersen, Lars G. M. Pettersson and Anders Nilsson, *Stability of Pt-modified Cu(111) in the presence of oxygen and its implication on the overall electronic structure*, J. Phys. Chem. C **117**, 16371-16380 (2013).
270. Yoshihisa Harada, Takashi Tokushima, Yuka Horikawa, Osamu Takahashi, Hideharu Niwa, Masaki Kobayashi, Masaharu Oshima, Yasunori Senba, Haruhiko Ohashi, Kjartan Thor Wikfeldt, Anders Nilsson, Lars G. M. Pettersson and Shik Shin, *Selective Probing of OH/OD Stretch Vibrations in Liquid Water using Resonant Inelastic Soft X-ray Scattering*, Phys. Rev. Letters **111**, 193001 (2013).
271. Lars Gunnar Moody Pettersson and Anders Nilsson, *A Molecular Perspective on the d-band Model; Synergy between Experiment and Theory*, Topics in Catalysis **57**, 2-13 (2014).
272. J. A. Sellberg, C. Huang, T. A. McQueen, N. D. Loh, H. Laksmono, D. Schlesinger, R. G. Sierra, D. Nordlund, C. Y. Hampton, D. Starodub, D. P. DePonte, M. Beye, C. Chen, A. V. Martin, A. Barty, K. T. Wikfeldt, T. M. Weiss, C. Caronna, J. Feldkamp, L. B. Skinner, M. M. Seibert, M. Messerschmidt, G. J. Williams, S. Boutet, L. G. M. Pettersson, M. J. Bogan, and A. Nilsson, *Ultrafast X-ray probing of water structure below the homogeneous ice nucleation temperature*, Nature **510**, 381 (2014).
273. Iradwikanari Waluyo, Dennis Nordlund, Uwe Bergmann, Daniel Schlesinger, Lars G.M. Pettersson, and Anders Nilsson, *A Different View of Structure-Making and Structure-Breaking in Alkali Halide Aqueous Solutions through X-ray Absorption Spectroscopy*, J. Chem. Phys. **140**, 244506 (2014).
274. Jonas. A. Sellberg, Sarp Kaya, Vegard H. Segtnan, Chen Chen, Tolek Tyliszczak, Hirohito Ogasawara, Dennis Nordlund, Lars G. M. Pettersson, and Anders Nilsson, *Comparison of x-ray absorption spectra between water and ice: new ice data with low pre-edge absorption cross-section*, J. Chem. Phys. **141**, 034507 (2014).
275. Simon Schreck, Martin Beye, Jonas A. Sellberg, Trevor McQueen, Hartawan Laksmono, Daniel DePonte, Brian Kennedy, Sebastian Eckert, Daniel Schlesinger, Dennis Nordlund, Hirohito Ogasawara, Raymond G. Sierra, Vegard H. Segtnan, Katharina Kubiceck, William F. Schlotter, Georgi L. Dakovski, Stefan P. Moeller, Uwe Bergmann, Simone Techert, Lars G. M. Pettersson, Philippe Wernet, Michael J. Bogan, Yoshihisa Harada, Anders Nilsson, and Alexander Föhlisch, *Reabsorption of Soft X-ray Emission at High X-ray Free-Electron Laser Fluences*, Phys. Rev. Letters **113**, 153002 (2014).
276. Rasmus K.B. Karlsson, Heine Hansen, Thomas Bligaard, Ann Cornell, and Lars G.M. Pettersson, *Ti atoms in Ru<sub>0.3</sub>Ti<sub>0.7</sub>O<sub>2</sub> mixed oxides form active and selective sites for electrochemical chlorine evolution*, Electrochimica Acta **146**, 733-740 (2014).
277. Hernan G. Sanchez Casalongue, Jesse D. Benck, Charlie Tsai, Rasmus K. B. Karlsson, Sarp Kaya, May Ling Ng, Lars G.M. Pettersson, Frank Abild-Pedersen, J. K. Nørskov, Hirohito Ogasawara, Thomas F. Jaramillo and Anders Nilsson, *Operando Characterization of an Amorphous Molybdenum Sulfide Nanoparticle Catalyst during the Hydrogen Evolution Reaction*, J. Phys. Chem. C **118**, 29252–29259 (2014).
278. Jonas A. Sellberg, Trevor A. McQueen, Hartawan Laksmono, Simon Schreck, Martin Beye, Daniel P. DePonte, Brian O'Kennedy, Dennis Nordlund, Raymond G. Sierra, Daniel

Schlesinger, Takashi Tokushima, Iurii Zhovtobriukh, Sebastian Eckert, Vegard H. Segtnan, Hirohito Ogasawara, Katharina Kubicek, Simone Techert, Uwe Bergmann, Georgi L. Dakovski, William F. Schlotter, Yoshihisa Harada, Michael J. Bogan, Philippe Wernet, Alexander Föhlisch, Lars G. M. Pettersson, and Anders Nilsson, *X-ray Emission Spectroscopy of Bulk Liquid Water in “No-man’s Land”*, *J. Chem. Phys.* **142**, 044505 (2015).

- 279.** J. Gladh, H. Öberg, L. G. M. Pettersson and H. Öström, *Detection of Adsorbate Overlayer Structural Transitions Using Sum-Frequency Generation Spectroscopy*, *Surf. Sci.* **633**, 77-81 (2015).
- 280.** Lars G.M. Pettersson and Anders Nilsson, *The Structure of Water; from Ambient to Deeply Supercooled*, *J. Non-Crystalline Solids* **407**, 399-417 (2015).
- 281.** Rosalba Juarez-Mosqueda, Andreas Mavrandonakis, Agnieszka Kuc, Lars G. M. Pettersson, Thomas Heine, *Theoretical analysis of hydrogen spillover mechanism on carbon nanotubes*, *Front. Chem.* **3**, 00002 (2015).
- 282.** Chen Chen, Congcong Huang, Iradwikanari Waluyo, Thomas Weiss, Lars G.M. Pettersson and Anders Nilsson, *Long-Range Ion-Water and Ion-Ion Interactions in Aqueous Solutions*, *Phys. Chem. Chem. Phys.* **17**, 8427-8430 (2015).
- 283.** Osamu Takahashi, Mai Kimoto, and Lars G. M. Pettersson, *Theoretical study of the X-ray natural circular dichroism of some crystalline amino acids*, *Chem. Phys.* **450-451**, 109–114 (2015).
- 284.** H. Öström, H. Öberg, H. Xin, J. LaRue, M. Beye, M. Dell'Angela, J. Gladh, M. L. Ng, J. A. Sellberg, S. Kaya, G. Mercurio, D. Nordlund, M. Hantschmann, F. Hieke, D. Kühn, W. F. Schlotter, G. L. Dakovski, J. J. Turner, M. P. Minitti, A. Mitra, S. P. Moeller, A. Föhlisch, M. Wolf, W. Wurth, M. Persson, J. K. Nørskov, F. Abild-Pedersen, H. Ogasawara, L. G. M. Pettersson, A. Nilsson, *Probing the Transition State Region in Catalytic CO Oxidation on Ru*, *Science* **347**, 978-982 (2015); doi:10.1126/science.1261747
- 285.** H. Öberg, J. Gladh, M. Dell'Angela, T. Anniyev, M. Beye, R. Coffee, A. Föhlisch, T. Katayama, S. Kaya, J. LaRue, A. Møgelhøj, D. Nordlund, H. Ogasawara, W. F. Schlotter, J. A. Sellberg, F. Sorgenfrei, J. J. Turner, M. Wolf, W. Wurth, H. Öström, A. Nilsson, J. K. Nørskov, L. G. M. Pettersson, *Optical Laser-Induced CO Desorption from Ru(0001) Monitored with a Free-Electron X-ray Laser: DFT Prediction and X-ray Confirmation of a Precursor State*, *Surface Science* **640**, 80-88 (2015).
- 286.** H. Xin, J. LaRue, H. Öberg, M. Beye, M. Dell'Angela, J. Turner, J. Gladh, M. L. Ng, J. A. Sellberg, S. Kaya, G. Mercurio, D. Nordlund, W. F. Schlotter, A. Föhlisch, M. Wolf, W. Wurth, H. Ogasawara, J. K. Nørskov, H. Öström, L. G. M. Pettersson, A. Nilsson, F. Abild-Pedersen, *Strong Influence of Coadsorbate Interaction on CO Desorption Dynamics*, *Phys. Rev. Lett.* **114**, 156101 (2015).
- 287.** A. Nilsson, D. Schlesinger and L. G. M. Pettersson, *X-ray spectroscopy, scattering and simulation studies of instantaneous structures in water*, in *Water: Fundamentals as the Basis for Understanding the Environment and Promoting Technology*, Vol. 187. (eds. P.G. Debenedetti, M.A. Ricci & F. Bruni) (IOS Press, Amsterdam; 2015).

- 288.** Hartawan Laksmono, Trevor A. McQueen, Jonas A. Sellberg, N. Duane Loh, Congcong Huang, Daniel Schlesinger, Raymond G. Sierra, Christina Y. Hampton, Dennis Nordlund, Martin Beye, Andrew V. Martin, Anton Barty, M. Marvin Seibert, Marc Messerschmidt, Garth J. Williams, Sébastien Boutet, Katrin Amann-Winkel, Thomas Loerting, Lars G. M. Pettersson, Michael J. Bogan, and Anders Nilsson, *Anomalous Behavior of the Homogeneous Ice Nucleation Rate in “No-Man’s Land”*, *J. Phys. Chem. Letters* **6**, 2826–2832 (2015).
- 289.** H. Öberg, J. Gladh, K. Marks, H. Ogasawara, A. Nilsson, L. G. M. Pettersson and H. Öström, *Indication of non-thermal contribution to visible femtosecond laser-induced CO oxidation on Ru(0001)*, *J. Chem. Phys.* **143**, 074701 (2015).
- 290.** Rasmus K. B. Karlsson, Ann Cornell and Lars G. M. Pettersson, *The electrocatalytic properties of doped TiO<sub>2</sub>*, *Electrochimica Acta* **180**, 514–527 (2015).
- 291.** Anders Nilsson and Lars G.M. Pettersson, *The Structural Origin of Anomalous Properties of Liquid Water*, *Nature Commun.* **6**, 8998 (2015).
- 292.** Thomas Fransson, Iurii Zhovtobriukh, Sonia Coriani, Kjartan Thor Wikfeldt, Patrick Norman, and Lars G. M. Pettersson, *Requirements on first-principles calculations of X-ray absorption spectra of liquid water*, *Phys. Chem. Chem. Phys.* **18**, 566 – 583 (2016).
- 293.** Valeriy Pogorelov, Yelyzaveta Chernolevska, Yevhenii Vaskivskyi, Lars G.M. Pettersson, Iryna Doroshenko, Valdas Sablinskas, Vytautas Balevicius, Justinas Ceponkus, Kristina Kovaleva, Alex Malevich, George Pitsevich, *Structural transformations in bulk and matrix-isolated methanol from measured and computed infrared spectroscopy*, *J. Mol. Liq.* **216**, 53–58 (2016).
- 294.** Daniel Schlesinger, Jonas A. Sellberg, Anders Nilsson and Lars G. M. Pettersson, *Evaporative cooling of microscopic water droplets in vacuo: Molecular dynamics simulations and kinetic gas theory*, *J. Chem. Phys.* **144**, 124502 (2016).
- 295.** George Pitsevich, Iryna Doroshenko, Lars G. M. Pettersson, Valdas Sablinskas, and V. Balevicius, *Combinatorial mechanism of broadening of the O-H stretching bands in hydrogen-bonded molecular clusters*, *J. Appl. Spectroscopy* **83**, 350-357 (2016).
- 296.** A. Nilsson, S. Schreck, F. Perakis, L.G.M. Pettersson, *Probing Water with X-ray Lasers*, *Advances in Physics X* **1**, 226-245 (2016). DOI: 10.1080/23746149.2016.1165630.
- 297.** Rasmus K. B. Karlsson, Ann Cornell, and Lars G. M. Pettersson, *Structural Changes in RuO<sub>2</sub> During Electrochemical Hydrogen Evolution*, *J. Phys. Chem. C* **120**, 7094–7102 (2016). 10.1021/acs.jpcc.5b11696
- 298.** A. Nilsson, D. Schlesinger and L. G. M. Pettersson, *X-ray and simulation studies of water*, *Rivista del Nuovo Cimento* **39**, 225-278 (2016).
- 299.** P. Gallo, K. Amann-Winkel, C. A. Angell, M. A. Anisimov, F. Caupin, C. Chakravarty, T. Loerting, A. Z. Panagiotopoulos, J. Russo, H. Tanaka, J. A. Sellberg, H. E. Stanley, E. Lascaris, C. Vega, L. Xu, L. G. M. Pettersson, *Water: A Tale of Two Liquids*, *Chem. Rev.* **116**, 7463-7500 (2016). <http://dx.doi.org/10.1021/acs.chemrev.5b00750>

- 300.** Thomas Fransson, Yoshihisa Harada, Nobuhiru Kosugi, Nicholas A. Besley, Bernd Winter, John Rehr, Lars G.M. Pettersson and Anders Nilsson, *X-ray and Electron Spectroscopy of Water*, Chem. Rev. **116**, 7551–7569 (2016).
- 301.** Lars Gunnar Moody Pettersson, Richard Henchman, Anders Nilsson, *Introduction: Water the most anomalous liquid*, Chem. Rev. **116**, 7459–7461 (2016).
- 302.** Daniel Schlesinger, K. Thor Wikfeldt, Lawrie B. Skinner, Chris J. Benmore, Anders Nilsson and Lars G. M. Pettersson, *The temperature dependence of intermediate range oxygen-oxygen correlations in liquid water*, J. Chem. Phys. **145**, 084503 (2016).
- 303.** M. Beye, H. Öberg, H. Xin, G. L. Dakovski, M. Dell'Angela, A. Föhlisch, J. Gladh, M. Hantschmann, F. Hieke, S. Kaya, D. Kühn, J. LaRue, G. Mercurio, M. P. Miniti, A. Mitra, S. P. Möller, M. L. Ng, A. Nilsson, D. Nordlund, J. Nørskov, H. Öström, H. Ogasawara, M. Persson, W. F. Schlötter, J. A. Sellberg, M. Wolf, F. Abild-Pedersen, L. G. M. Pettersson, and W. Wurth, *Chemical Bond Activation Observed with an X-ray Laser*, J. Phys. Chem. Lett. **7**, 3647–3651 (2016).
- 304.** H. Pathak, J. C. Palmer, D. Schlesinger, K. T. Wikfeldt, J. A. Sellberg, L.G.M. Pettersson and A. Nilsson, *The structural validity of various thermodynamical models of supercooled water*, J. Chem. Phys. **145**, 134507 (2016).
- 305.** V. Pogorelov, I. Doroshenko, G. Pitsevich, V. Balevicius, V. Sablinskas, B. Krivenko, L.G.M. Pettersson, *From Clusters to Condensed Phase – FT IR Studies of Water*, J. Mol. Liq. **235**, 7–10 (2017).
- 306.** G. Pitsevich, I. Doroshenko, A. Malevich, E. Shalamberidze, V. Saposhko, V. Pogorelov, L.G.M. Pettersson, *Temperature dependence of the intensity of the vibration-rotational absorption band  $\nu_2$  of  $H_2O$  trapped in an argon matrix*, Spectrochimica Acta A **172**, 83–90 (2017). doi: 10.1016/j.saa.2016.04.028
- 307.** André Eilert, Filippo Cavalca, F. Sloan Roberts, Jürg Osterwalder, Chang Liu, Marco Favaro, Ethan J. Crumlin, Hirohito Ogasawara, Daniel Friebel, Lars G. M. Pettersson, and Anders Nilsson, *Subsurface Oxygen in Oxide-Derived Copper Electrocatalysts for Carbon Dioxide Reduction*, J. Phys. Chem. Lett. **8**, 285–290 (2017).
- 308.** A. Nilsson, J. LaRue, H. Öberg, H. Ogasawara, M. Dell'Angela, M. Beye, H. Öström, J. Gladh, J.K. Nørskov, W. Wurth, F. Abild-Pedersen, L.G.M. Pettersson, *Catalysis in Real Time using X-ray Lasers*, Chem. Phys. Letters (FRONTIERS) **675**, 145–173 (2017).
- 309.** G. Pitsevich, A. Malevich, E. Kozlovskaya, E. Mahnach, I. Doroshenko, V. Pogorelov, Lars G.M. Pettersson, V. Sablinskas, V. Balevicius, *MP4 Study of the Anharmonic Coupling of the Shared Proton Stretching Vibration of the Protonated Water Dimer in Equilibrium and Transition States*, J. Phys. Chem. A **121**, 2151–2165 (2017).
- 310.** M. P. Ljungberg, I. Zhovtobriukh, O. Takahashi, and L. G. M. Pettersson, *Core-hole-induced dynamical effects in the x-ray emission spectrum of liquid methanol*, J. Chem. Phys. **146**, 134506 (2017).

- 311.** Egon Campos Dos Santos, Maicon Pierre Lourenço, Lars G. M. Pettersson, and Hélio Anderson Duarte, *Stability, structure, and electronic properties of the pyrite/arsenopyrite solid-solid interface – a DFT study*, J. Phys. Chem. C **121**, 8042–8051 (2017).
- 312.** A. S. de Wijn and L. G. M. Pettersson, *How square ice helps lubrication*, Phys. Rev. B **95**, 165433 (2017).
- 313.** G. Pitsevich, E. Shalamberidze, A. Malevich, V. Sablinskas, V. Balevicius, L.G.M. Pettersson, *Calculation of the Vibration-Rotational Transition Intensities of Water Molecules Trapped in an Argon Matrix: Stretching O-H Vibrations Spectral Region*, Mol. Phys. **115**, 2605–2613 (2017).
- 314.** F. Perakis, K. Amann-Winkel, F. Lehmkuhler, M. Sprung, D. Pettersson, J. A. Sellberg, H. Pathak, A. Späh, F. Cavalca, D. Schlesinger, A. Ricci, A. Jain, B. Massani, F. Aubree, C. J. Benmore, T. Loerting, G. Grübel, L. G. M. Pettersson and A. Nilsson, *Diffusive dynamics during the high- to low-density transition in amorphous ices*, Proc. Natl. Acad. Sci. **114**, 8193–8198 (2017).
- 315.** Kyung Hwan Kim, Harshad Pathak, Alexander Späh, Fivos Perakis, Daniel Pettersson, Jonas A. Sellberg, Tetsuo Katayama, Yoshihisa Harada, Hirohito Ogasawara, Lars G.M. Pettersson, Anders Nilsson, *Temperature-Independent Nuclear Quantum Effects on the Structure of Water*, Phys. Rev. Lett. **119**, 075502 (2017).
- 316.** J. LaRue, O. Krejci, L. Yu, M. Beye, M. L. Ng, H. Öberg, H. Xin, G. Mercurio, S. Moeller, J. J. Turner, D. Nordlund, R. Coffee, M. P. Minitti, W. Wurth, L. G. M. Pettersson, H. Öström, A. Nilsson, F. Abild-Pedersen, H. Ogasawara, *Real-Time Elucidation of Catalytic Pathways in CO Hydrogenation on Ru*, J. Phys. Chem. Lett. **8**, 3820–3825 (2017).
- 317.** Chang Liu, Maicon P. Lourenço, Filippo Cavalca, Oscar Diaz-Morales, Hélio A. Duarte, Anders Nilsson and Lars G. M. Pettersson, *Stability and Effects of Subsurface Oxygen in Oxide-Derived Cu Catalyst for CO<sub>2</sub> Reduction*, J. Phys. Chem. C **121**, 25010–25017 (2017).
- 318.** Filippo Cavalca, Rafael Ferragut, Stefano Aghion, André Eilert, Oscar Diaz-Morales, Chang Liu, Ai-Leen Koh, Thomas W. Hansen, Lars G. M. Pettersson, and Anders Nilsson, *Nature and distribution of stable subsurface oxygen in copper electrodes during electrochemical CO<sub>2</sub> reduction*, J. Phys. Chem. C **121**, 25003–25009 (2017).
- 319.** Y. Harada, J. Miyawaki, H. Niwa, K. Yamazoe, L. G. M. Pettersson and A. Nilsson, *Probing the OH Stretch in Different Local Environments in Liquid Water*, J. Phys. Chem. Lett. **8**, 5487–5491 (2017).
- 320.** Osamu Takahashi, Mathias P. Ljungberg, Lars G. M. Pettersson, *X-ray Emission Spectrum of Liquid Ethanol – Origin of Split Peaks*, J. Phys. Chem. B **121**, 11163–11168 (2017).
- 321.** Francisco A. Delesma, Maxime Van den Bossche, Henrik Grönbeck, Patrizia Calaminici, Andreas M. Köster, and Lars G.M. Pettersson, *A Chemical View on X-ray Photoelectron Spectroscopy: the ESCA molecule and surface-to-bulk XPS shifts*, ChemPhysChem **19**, 169 – 174 (2018).

- 322.** Iurii Zhovtobriukh, Nicholas A. Besley, Thomas Fransson, Anders Nilsson, and Lars G.M. Pettersson, *Relationship between X-Ray Emission and Absorption Spectroscopy and the Local H-bond Environment in Water*, J. Chem. Phys. **148**, 144507 (2018).
- 323.** Fivos Perakis, Gaia Camisasca, Thomas J. Lane, Alexander Späh, Kjartan Thor Wikfeldt, Jonas A. Sellberg, Felix Lehmkuhler, Harshad Pathak, Kyung Hwan Kim, Katrin Amann-Winkel, Simon Schreck, Sanghoon Song, Takahiro Sato, Marcin Sikorski, Andre Eilert, Trevor McQueen, Hirohito Ogasawara, Dennis Nordlund, Wojciech Roseker, Jake Koralek, Silke Nelson, Philip Hart, Roberto Alonso-Mori, Yiping Feng, Diling Zhu, Aymeric Robert, Gerhard Grüberl, Lars G. M. Pettersson, and Anders Nilsson, *Coherent X-rays reveal the influence of cage effects on ultrafast water dynamics*, Nature Commun. **9**, 1917 (2018).
- 324.** Svante Hedström, Egon Campos dos Santos, Chang Liu, Karen Chan, Frank Abild-Pedersen, Lars G. M. Pettersson, *Spin uncoupling in chemisorbed ethylenedione and carbon dioxide – two high-energy intermediates in catalytic carbon-dioxide reduction*, J. Phys. Chem. C **122**, 12251–12258 (2018).
- 325.** Daniel Mariedahl, Fivos Perakis, Alexander Späh, Harshad Pathak, Kyung Hwan Kim, Gaia Camisasca, Daniel Schlesinger, Chris Benmore, Lars Gunnar Moody Pettersson, Anders Nilsson and Katrin Amann-Winkel, *X-ray Scattering and O-O Pair-Distribution Functions of Amorphous Ices*, J. Phys. Chem. B **122**, 7616–7624 (2018).
- 326.** Guilherme Ferreira de Lima, Hélio Anderson Duarte and Lars G. M. Pettersson, *X-ray Absorption Spectroscopy Calculations on Pristine and Modified Chalcopyrite Surfaces*, J. Phys. Chem. C **122**, 20200–20209 (2018).
- 327.** Simon Schreck, Elias Diesen, Jerry LaRue, Hirohito Ogasawara, Kess Marks, Dennis Nordlund, Matthew Weston, Martin Beye, Filippo Cavalca, Fivos Perakis, Jonas Sellberg, Andre Eilert, Kyung Hwan Kim, Giacomo Coslovich, Ryan Coffee, Jacek Krzywinski, Alex Reid, Stefan Moeller, Alberto Lutman, Henrik Öström, Lars G. M. Pettersson, and Anders Nilsson, *Atom-Specific Activation in Catalytic CO Oxidation*, J. Chem. Phys. **149**, 234707 (2018).
- 328.** Iurii Zhovtobriukh, Patrick Norman, Lars G. M. Pettersson, *X-ray Absorption Spectrum Simulations of Hexagonal Ice*, J. Chem. Phys. **150**, 034501 (2019).
- 329.** Chang Liu, Svante Hedström, Joakim H. Stenlid, and Lars G. M. Pettersson, *Amorphous, Periodic Model of a Copper Electrocatalyst with Subsurface Oxygen for Enhanced CO Coverage and Dimerization*, J. Phys. Chem. C **123**, 4961–4968 (2019).
- 330.** Joakim Halldin Stenlid, Egon Campos dos Santos, Adam Johannes Johansson, and Lars GM Pettersson, *On the Nature of the Cathodic Reaction During Corrosion of Copper in Anoxic Sulfide Solutions*, J. Electrochem. Soc. **166**, C196-C208 (2019).
- 331.** Lars G.M. Pettersson, *A Two-State Picture of Water and the Funnel of Life*, In: Bulavin L., Xu L. (eds) Modern Problems of the Physics of Liquid Systems. Springer Proceedings in Physics **223**, 3-39 (2019) Springer, Cham.

- 332.** Iurii Zhovtobriukh, Benedito J.C. Cabral, Carmelo Corsaro, Domenico Mallamace, Lars G. M. Pettersson, *Liquid Water Structure from X-ray Absorption and Emission, NMR Shielding and X-ray Diffraction*, *Science China* **62**, 107010 (2019).
- 333.** Gaia Camisasca, Nuno Galamba, Kjartan Thor Wikfeldt and Lars G.M. Pettersson, *Translational and Rotational Dynamics of High and Low Density TIP4P/2005 Water*, *J. Chem. Phys.* **150**, 224507 (2019).
- 334.** Gaia Camisasca, Daniel Schlesinger, Iurii Zhovtobriukh, George Pitsevich, Lars G.M. Pettersson, *A Proposal for the Structure of High- and Low-Density Fluctuations in Liquid Water*, *J. Chem. Phys.* **151**, 034508 (2019).
- 335.** Gaia Camisasca, Harshad Pathak, Kjartan Thor Wikfeldt and Lars G.M. Pettersson, *Radial distribution functions of water: models vs experiments*, *J. Chem. Phys.* **151**, 044502 (2019).
- 336.** Lars G.M. Pettersson, Yoshihisa Harada and Anders Nilsson, *Do X-ray spectroscopies provide evidence for continuous distribution models of water at ambient conditions?*, *Proc. Natl. Acad. Sci. (USA)* **116**, 17156-17157 (2019).
- 337.** Hsin-Yi Wang, Simon Schreck, Matthew Weston, Chang Liu, Hirohito Ogasawara, Jerry LaRue, Fivos Perakis, Martina Dell'Angela, Flavio Capotondi, Luca Giannessi, Emanuele Pedersoli, Denys Naumenko, Ivaylo Nikolov, Lorenzo Raimondi, Carlo Spezzani, Martin Beye, Filippo Cavalca, Boyang Liu, Jörgen Gladh, Sergey Koroidov, Piter S. Miedema, Roberto Costantini, Lars G. M. Pettersson, and Anders Nilsson, *Time-Resolved Observation of Transient Precursor State of CO on Ru(0001) using Carbon K-edge spectroscopy*, *PhysChemChemPhys* **22**, 2677-2684 (2020).
- 338.** Svante Hedström, Joakim Halldin Stenlid, Chang Liu, and Lars G. M. Pettersson, *Photodriven CO Dimerization on Cu<sub>2</sub>O from an Electronic-Structure Perspective*, *Sustainable Energy & Fuels* **4**, 670 – 677 (2020).
- 339.** Joakim Halldin Stenlid, Egon Campos Dos Santos, Alexander Bagger, Adam Johannes Johansson, Jan Rossmeisl, Lars GM Pettersson, *The Electrochemical Interface During Corrosion of Copper in Anoxic Sulfide-Containing Groundwater – a Computational Study*, *J. Phys. Chem. C* **124**, 469-481 (2020).
- 340.** Maicon Pierre Lourenço, Egon Campos dos Santos, Lars G. M. Pettersson, and Hélio Anderson Duarte, *Accurate SCC-DFTB parameterization for bulk water*, *J. Chem. Theory Comp.* **16**, 1768-1778 (2020).
- 341.** G. A. Pitsevich, E. N. Kozlovskaya, A. E. Malevich, I. Yu. Doroshenko, V. S. Satsunkevich, and Lars G. M. Pettersson, *Some useful correlations for H-bonded systems*, *Molecular Crystals and Liquid Crystals* **696**, 15-28 (2020).
- 342.** Mikael Valter, Egon Campos dos Santos, Lars G. M. Pettersson, and Anders Hellman, *Partial Electrooxidation of Glycerol on Close-Packed Transition Metal Surfaces: Insights from First-Principles Calculations*, *J. Phys. Chem. C* **124**, 17907–17915 (2020).
- 343.** Alexander Holm, Emmett D. Goodman, Joakim Halldin Stenlid, Aisulu Aitbekova, Rosadriana Zelaya, Benjamin T. Diroll, Aaron Johnston-Peck, Kun-Che Kao, Curtis W. Frank,

Lars G. M. Pettersson, Matteo Cargnello, *Nanoparticle Spatial Distribution Controls Catalyst Activity and Stability*, J. Am. Chem. Soc. **142**, 14481-14494 (2020).

- 344.** Rafael B. Araujo, Daniel Martín-Yerga, Egon Campos dos Santos, Ann Cornell, Lars G. M. Pettersson, *Elucidating the Role of Ni to Enhance the Methanol Oxidation Reaction on Pd Electrocatalysts*, Electrochimica Acta **360**, 136954 (2020).
- 345.** Eric L. Shirley, Lars G.M. Pettersson and David G. Prendergast, *Core-hole potentials and related effects*, IUCr Handbook 9, Chapter 2.17, accepted.
- 346.** Joakim Halldin Stenlid, Egon Campos dos Santos, Rosa M. Arán Ais, Alexander Bagger, Adam Johannes Johansson, Beatriz Roldan Cuenya, Jan Rossmeisl, Lars Gunnar Moody Pettersson, *Uncovering the Electrochemical Interface of Low-Index Copper Surfaces in Deep Groundwater Environments*, Electrochimica Acta **362**, 137111 (2020).
- 347.** Elias Diesen, Gabriel L. S. Rodrigues, Alan Luntz, Frank Abild-Pedersen, Lars G. M. Pettersson, Johannes Voss, *Accuracy of XAS theory for unravelling structural changes of adsorbates: CO on Ni(100)*, AIP Advances **10**, 115014 (2020).
- 348.** Joakim Halldin Stenlid, Egon Campos dos Santos, Adam Johannes Johansson, Lars GM Pettersson, *Properties of Interfaces Between Copper and Copper Sulphide/Oxide Films*, Corrosion Science **183**, 109313 (2021).
- 349.** Mikael Valter, Egon Campos dos Santos, Lars G. M. Pettersson, and Anders Hellman, *Selectivity of the First Two Glycerol Dehydrogenation Steps Determined Using Scaling Relationships*, ACS Catalysis **11**, 3487–3497 (2021).
- 350.** Sergey Koroidov, Anna Winiwarter, Oscar Diaz-Morales, Mikaela Görlin, Joakim Halldin Stenlid, Hsin-Yi Wang, Mia Börner, Christopher Goodwin, Markus Soldemo, Lars Gunnar Moody Pettersson, Jan Rossmeisl, Tony Hansson, Ib Chorkendorff, and Anders Nilsson, *Chemisorbed Oxygen or Surface Oxides Steer the Selectivity in Pd Electrocatalytic Propene Oxidation Observed by Operando Pd L-edge X-ray Absorption Spectroscopy*, Catalysis Science & Technology **11**, 3347-3352 (2021).

## Submitted Manuscripts – Under Revision

Rafael B. Araujo, Gabriel L. S. Rodrigues, Egon Campos dos Santos, Lars G. M. Pettersson, *Adsorption Energies on Transition Metal Surfaces: Towards an Accurate and Balanced Description*, submitted to Nature Commun.

## Submitted Manuscripts

Xiaowen Yu, Egon Campos dos Santos, Jai White, Germán Salazar-Alvarez, Lars G.M. Pettersson, Ann Cornell, and Mats Johnsson, *Electrocatalytic glycerol oxidation with concurrent hydrogen evolution utilizing an efficient catalyst based on Pt trapped at vacancies of MoO<sub>x</sub>*, submitted to Advanced Functional Materials.

Egon Campos dos Santos, Rafael B. Araujo, Mikael Valter, German Salazar-Alvarez, Mats Johnsson, Michal Bajdich, Frank Abild-Pedersen, Lars Gunnar Moody Pettersson, *Efficient*

Lars G.M. Pettersson

*Screening of Bi-Metallic Electrocatalysts for Glycerol Valorization*, submitted to *Electrochimica Acta*.

Lars G.M. Pettersson and Osamu Takahashi, *X-ray Emission Spectroscopy – A Genetic Algorithm to Disentangle Core-Hole-Induced Dynamics*, submitted to *Theor. Chem. Acc.*

## Pedagogical Contributions

1. L.G.M. Pettersson, *Kvantmekanik och Kvantkemi (Quantum Mechanics and Quantum Chemistry)*, in Swedish. Course material (62 pages) for course on Computer Chemistry, Chemistry Department, Stockholm University, 1997.
2. G. Edvinsson, K.E. Johansson and L.G.M. Pettersson, *Implementation of Computer Aided Learning in Undergraduate Physics Teaching*, USIP Report 97-08, 1997.
3. I. Cohen, G. Edvinsson, CH. Johannesson, K.E. Johansson, L.G.M. Pettersson and P. Sällström, *Flexible Learning in Undergraduate Physics and Mechanics*, USIP Report 2001-04, 2001.