

Bibliography

- [1] F. Bozso, G. Ertl, M. Grunze, M. Weiss; *Interaction of nitrogen with iron surfaces. I. Fe(100) and Fe(111)*; J. Catal. **49** (1977) 18-41
- [2] F. Bozso, G. Ertl, M. Weiss; *Interaction of nitrogen with iron surfaces. II. Iron(110)*; J. Catal. **50** (1977) 519-529
- [3] G. Ertl; *Surface Science and catalysis- Studies on the mechanism of ammonia synthesis: The P.H. Emmett award address*; Catal. Rev. Sci. Eng. **21** (1980) 201-223
- [4] C. Bokhoven, C. van Heerden, R. Westrick, P. Zwietering; *Research on ammonia synthesis since 1940, in Catalysis, vol. III*; Ed. P.H. Emmet (1955) Reinhold, New York
- [5] R.L.Toomes, J.-H.Kang, D.P.Woodruff, M.Polcik, M.Kittel, J.-T.Hoeft; *Can glycine form homochiral structural domains on low-index copper surfaces?*; Surf. Sci. **522** (2003) L9-L14
- [6] R. Smoluchowski; *Anisotropy of the electronic work function of metals*; Phys. Rev. **60** (1941) 661-674
- [7] B.H. Bransden and C.J. Joachain; *Physics of atoms and molecules*; Ed. Longman Scientific and Technical (1992) England
- [8] V.Fritzsche and P.Rennert; *A reduced angular momentum expansion in the multiple-scattering theory*; Phys. Stat. Sol.(b)**135** (1986) 49-61
- [9] V.Fritzsche; *Approximations for photoelectron scattering*; Surf. Sci. **213** (1989) 648-656
- [10] V.Fritzsche; *A new spherical-wave approximation for photoelectron diffraction, EX-AFS and MEED*; J.Phys.: Condensed Matter **2** (1990) 1413-1424
- [11] V.Fritzsche; *Calculation of Auger-electron diffraction at a Ni(111) surface*; J.Phys.: Condensed Matter **2** (1990) 9735-9747
- [12] V.Fritzsche; *Consequences of a finite-energy resolution for photoelectron diffraction spectra*; Surf. Sci. **265** (1992) 187-195

- [13] V.Fritzsche, K.-M.Schindler, P.Gardner, A.M.Bradshaw, M.C.Asensio and D.P.Woodruff; *The effect of anisotropic molecular vibrations in photoelectrons diffraction adsorbed species*; Surf. Sci. **269/270** (1992) 35-40
- [14] V.Fritzsche and J.B. Pendry; *Linear-superposition method for the multiple-scattering problem in low-energy-photoelectron diffraction*; Phys. Rev. B **48** (1993) 9054-9057
- [15] M. Kittel; *Analyse von Oberflaechenstrukturen mit Photoelektronenbeugung*; Doktorarbeit, Freie Universitaet Berlin, 2001
- [16] J.-T. Hoeft; *Structure investigation of adsorbates on surfaces using photoelectron diffraction*; PhD Thesis, Warwick University, 2003
- [17] P. Hofmann and K.M. Schindler; *Direct adsorbate-structure determination by scanned-energy-mode photoelectron diffraction*; Phys. Rev. B **47** (1993) 13941-13943
- [18] V.Fritzsche and D.P. Woodruff; *Direct photoelectron-diffraction method for adsorbate structural determinations*; Phys. Rev. B **46** (1992) 16128-16134
- [19] J.B. Pendry; *Reliability factors for LEED calculations*; J. Phys.: Condens. Matter **13** (1980) 937-944
- [20] <<http://www.bessy.de>>
- [21] S. Sasaki, K. Miyata and T. Takada; *A new undulator for generating variably polarized radiation*; Jpn. J. Appl. Phys. 2 **31**(12B) (1992) L1794-L1796
- [22] L. Pauling; *The nature of chemical bond*; Ed. Cornell University Press (1960) Ithaca, NY
- [23] K.A.R. Mitchell; *Analysis of surface bond lengths reported for chemisorption on metal surfaces*; Surf. Sci. **149** (1985) 93-104
- [24] K.A.R. Mitchell, S.A. Schlatter and R.N.S. Sodhi; *Further analysis of surface bond lengths measured for chemisorption on metal surfaces*; Can. J. Chem. **64** (1986) 1435-1439
- [25] C.R. Brundle, P.S. Bagus, D. Menzel and K. Hermann; *Adsorption of molecular nitrogen on nickel. II. Comparison of photoemission for N₂/Ni(100) to CO/Ni(100) and to theory*; Phys. Rev. B **24**, 12 (1981) 7041-7055
- [26] C.M. Kao and R.P. Messner; *Ab initio cluster-model study of the electronic ground-state and photoemission properties of NiN₂ and NiCO: Models of chemisorption*; Phys. Rev. B **31**, 8 (1985) 4825-4847
- [27] P.S. Bagus, C.R. Brundle, K. Hermann and D. Menzel; *Photoemission and theoretical studies of the electronic structure of molecular nitrogen on nickel*; Phys. Rev. B **24**, 12 (1980) 7041-7055

- [28] E. Umbach; *On the interpretation of XPS lines of weakly chemisorbed N₂ on transition metals*; Solid State Comm. **51**, 6 (1984) 365-369
- [29] H.-J. Freund, R.P. Messmer, C.M. Kao and E.W. Plummer; *Interpretation of the N 1s photoelectron spectra of chemisorbed N₂ in terms of local molecule-metal interactions*; Phys. Rev. B **31**, 8 (1985) 7041-7055
- [30] A. Nilsson, H. Tillborg and N. Maertensson; *Electronic structure of adsorbates from core-level shake-up spectra: N₂ on Ni(100)*; Phys. Rev. Lett. **67**, 8 (1991) 1015-1018
- [31] P. Decleva and M. Ohno; *Many-body calculation of the XPS core hole spectra of NiN₂*; Chem. Phys. **160** (1992) 341-351
- [32] P. Decleva and M. Ohno; *Giant satellite in the X-ray photoelectron spectroscopy core-hole spectra of adsorbates*; J. Chem. Phys. **96**, 11 (1992) 8120-8127
- [33] M. Ohno and P. Decleva; *New interpretation of the core hole spectra of CO and N₂ adsorbed on a Ni metal surface*; Surf. Sci. **269/270** (1992) 264-269
- [34] H. Tillborg, A. Nilsson, N. Maertensson; *Shake-up and shake-off structures in core level photoemission spectra from adsorbates*; J.Electr. Spectros. Rel. Phenom. **62** (1993) 73-93
- [35] M. Ohno, P. Decleva and G. Fronzoni; *Many-body calculations of the core excitation spectra of N₂ and NiN₂: Inequivalent N atoms and disappearance of the giant shake-up satellite in NiN₂*; Surf. Sci. **284** (1993) 372-382
- [36] M. Ohno, P. Decleva; *On the resonantly core excited states of the N₂/Ni and related systems*; Surf. Sci. **296** (1993) 87-96
- [37] E.J. Moler, S.A. Kellar, W.R.A. Huff, Z. Hussain, Y. Zheng, E.A. Hudson, Y. Chen, D.A. Shirley; *Adsorption site and structure determination of c(2x2) N₂/Ni(100) using angle-resolved photoemission extended fine structure*; Chem. Phys. Lett. **264** (1997) 502-507
- [38] N.V. Dobrodey, L.S. Cederbaum and F. Tarantelli; *Dynamical core-hole screening in weak chemisorption systems*; Phys. Rev. B **57**, 12 (1998) 7340-7351
- [39] N.V. Dobrodey, L.S. Cederbaum and F. Tarantelli; *Strong dynamical screening in weak chemisorption systems*; Surf. Sci. **402-404** (1998) 508-512
- [40] N.V. Dobrodey, L.S. Cederbaum and F. Tarantelli; *Partial localization of core holes in nonsymmetrical systems*; Phys. Rev. B **58**, 4 (1998) 2316-2323
- [41] M. Grunze, P.A. Dowben, R.G. Jones; *Thermodynamic measurements for N₂ adsorption on Ni(100)*; Surf. Sci. **141** (1984) 455-472

- [42] J. Stöhr and R. Jaeger; *Absorption-edge resonances, core-hole screening, and orientation of chemisorbed molecules: CO, NO and N₂ on Ni(100)*; Phys. Rev. B **26**, 8 (1982) 4111-4131
- [43] P.A. Dowben, Y. Sakisaka and T.N. Rhodin; *Angle-resolved photoemission from molecular N₂ adsorbed on Ni(100)*; Surf. Sci. **147** (1984) 89-102
- [44] W.F. Egelhoff, Jr.; *N₂ on Ni(100) angular dependence of the N 1s XPS peaks*; Surf. Sci. Lett. **141** (1984) L324-L328
- [45] W.F. Egelhoff, Jr.; *X-ray photoelectron and Auger-electron forward scattering - A new tool for surface crystallography*; Crit. Rev. Solid State Mat. Sci. **16** (1990) 213-235
- [46] W.F. Egelhoff, Jr.; *Core-level binding-energy-shift analysis of adsorption and dissociation*; Phys. Rev. B **29**, 6 (1984) 3681-3683
- [47] R.M. Lambert and M.E. Bridge; *The Chemical Physics of Solid Surfaces and Heterogenous Catalysis*; Ed. D.A. King and D.P. Woodruff (1984) Elsevier, New York
- [48] S. Varma and P.A. Dowben; *The effect of lateral interactions on the thermal desorption of N₂ from Ni(100)*; J. Vac. Sci. Technol. A **8**, 3 (1990) 2605-2609
- [49] T. Takaoka, M. Terahara, I. Kusunoki; *Collision-induced desorption of N₂ on Ni(100) studied with Fourier transform infrared spectroscopy*; Surf. Sci. **454-456** (2000) 218-221
- [50] J. Yoshinobu, R. Zenobi, J. Xu, Z. Xu, J.T. Yates, Jr.; *N₂ chemisorption on Ni(111): An infrared investigation under steady-state conditions*; J. Chem. Phys. **95** (1991) 9393-9400
- [51] G. Blyholder; *Molecular orbital view of chemisorbed carbon monoxide*; J. Phys. Chem. **68**, 10 (1964) 2772-2778
- [52] J.A. Rayne and W.G. Kemp; Phil. Mag. **1** (1956) 918
- [53] A.U. MacRae and L.H. Germer; *Thermal vibrations of surface atoms*; Phys. Rev. Lett. **8**, 12 (1962) 489-490
- [54] M.-C. Desjonqueres and D. Spanjaard; *Concepts in surface physics*, Ed. Springer-Verlag (1998) Berlin, Heidelberg, New York
- [55] A.U. MacRae; *Adsorption of oxygen on the (111), (100) and (110) surfaces of clean nickel*; Surf. Sci. **1** (1964) 319-348
- [56] T. Yokoyama, H. Hamamatsu, Y. kitajima, Y. Takata, S. Yagi, T. Ohta; *Vibrational and anharmonic properties of the surface S-Ni bonds in c(2x2)S/Ni(100) and c(2x2)S/Ni(110)*; Surf. Sci. **313** (1994) 197-208

- [57] R. Dippel, K.-U. Wiess, K.-M. Schindler, D.P. Woodruff, P. Gardner, V. Fritzsche, A.M. Bradshaw, M.C. Asensio; *Multiple sites coincidences and their resolution in photoelectron diffraction: PF₃ adsorbed on Ni(111)*; Surf. Sci. **287/288** (1993) 465-470
- [58] S. Andersson, J.B. Pendry; *Multiple coincidence in surface structure determinations*; Solid State Comm. **16**, 5 (1975) 563-566
- [59] S.W. Robey, J.J. Barton, C.C. Bahr, G. Liu, D.A. Shirley; *Angle-resolved-photoemission extended-fine-structure spectroscopy investigation of c/2x2)S/Ni(011)*; Phys. Rev. B **35**, 3 (1987) 1108-1121
- [60] P. Bennich, T. Wiell, O. Karis, M. Weinelt, N. Wassdahl, A. Nilsson, M.Nyberg, L.G.M. Pettersson, J. Stöhr, M. Samant; *Nature of the surface chemical bond in N₂ on Ni(100) studied by x-ray-emission spectroscopy and ab initio calculations*; Phys. Rev. B **57**, 15 (1998) 9274-9284
- [61] A. Nilsson, J. Hasselström, A. Föhlsich, O. Karis, L.G.M. Pettersson, M. Nyberg, L. Triguero; *Probing chemical bonding in adsorbates using X-ray emission spectroscopy*; J. Electron Spectroscopy and related phenomena **110-111** (2000) 15-39
- [62] D.I. Sayago, M. Kittel, J.T. Hoeft, M. Polcik, M. Pascal, C.L.A. Lamont, R.L. Toomes, J. Robinson, D.P. Woodruff; *The structure of the Ni(100)c(2x2)-N₂ surface: a chemical-state-specific scanned-energy mode photoelectron diffraction determination*; Surf. Sci. **538** (2003) 59-75
- [63] M.C. Payne, M.P. Teter, D.C. Allen, T.A. Arias, J.D. Joannopoulos; *Iterative minimization techniques for ab-initio total-energy calculations: molecular dynamics and conjugate gradients*; Rev. Mod. Phys. **64** (1992) 1045-1097
- [64] CASTEP 4.2 Academic version under UKCP-MSI agreement (1999)
- [65] Molecular Simulations Inc. available from <<http://www.msi.com>>
- [66] J.T. Hoeft, M. Polcik, D.I. Sayago, M. Kittel, R. Terborg, R.L. Toomes, J. Robinson, D.P. Woodruff, M. Pascal, G. Nisbet, C.L.A. Lamont; *Local adsorption sites and bondlength changes in Ni(100)/H/CO and Ni(100)/CO*; Surf. Sci. **540** (2003) 441-456
- [67] E. Umbach; *Satellite structures in photoemission spectra from different types of adsorbates*; Surf. Sci. **117** (1982) 482-502
- [68] P.R. Norton, R.L. Tapping, J.W. Goodale; *X-ray and filtered UV photoelectron spectroscopic study of CO adsorbed on Ni(100) and (111) surfaces*; Chem. Phys. Lett. **41**, 2 (1976) 247-251

- [69] H. Antonsson, A. Nilsson, N. MArtensson, I. Panas, P.E.M. Siegbahn; *Vibrational motion and geometrical structure in adsorbed CO studied by core level photoemission spectroscopy*; J. Electron Spectrosc. Relat. Phenom. **54-55** (1990) 601-613
- [70] A. Sandell, P. Bennich, A. Nilsson, B. Hernnas, O. Bjorneholm, N. Martensson; *Chemisorption of CO on Cu(100), Ag(110) and Au(110)*; Surf. Sci. **310** (1994) 16-26
- [71] K. Schönhammer and O. Gunnarsson; *Shape of core level spectra in adsorbates*; Solid State Communication **23** (1977) 691-693
- [72] K. Schönhammer and O. Gunnarsson; *Exactly soluble limits of a model for core level spectra of adsorbates*; Z. Phys. B **30**,3 (1978) 297-303
- [73] D.A. Shirley; *The effect of atomic and extra-atomic relaxation on atomic binding energies*; Chem. Phys. Lett. **16** (1972) 220-225
- [74] B. Gumhalter and D.M. Newns; *Relaxation shifts and plasmon excitation in adsorption spectroscopy of adsorbed atoms*; Phys. Lett. A **57** (1976) 423-425
- [75] N.D. Lang and A.R. Williams; *Core holes in chemisorbed atoms*; Phys. Rev. B **16** (1977) 2408-2419
- [76] G.H. Leigh, J.M. Murrell, W. Bremser, W.G. Proctor; ; Chem. Commun. 1661 (1970)
- [77] H. Binder and D. Sellmann; *ESCA studies on N₂-, N₂H₂-, N₂H₄- and NH₃-complexes of manganese*; Angew. Chem. **12** (1973) 1017-1019
- [78] B. Folkesson; *ESCA studies on the charge distribution in some dinitrogen complexes of rhenium, iridium, ruthenium, and osmium*; Acta Chem. Scand. **27** (1973) 287-302
- [79] J. Chatt, C.M. Elson, N.E. Hopper, G.L. Leigh; JCS Dalton 2392 (1975)
- [80] H.-J. Freund, H. Pulm, B. Dick, R. Lange; *X-ray photoemission study of satellite structure accompanying core ionization from coordinated nitrogen*; Chem. Phys. **81** (1983) 99-112
- [81] K.-M. Schindler, V. Fritzsche, M.C. Asensio, P. Gardner, D.E. Ricken, A.W. Robinson, A.M. Bradshaw, D.P. Woodruff, J.C. Conesa, A.R. Gonzlez-Elipe; *Structural determination of a molecular adsorbate by photoelectron diffraction: Ammonia on Ni(111)*; Phys. Rev. B **46** (1992) 4836-4843
- [82] Y. Zheng, E. Moler, E. Hudson, Z. Hussain, D.A. Shirley; *Structural determination of NH₃ adsorbed on Ni(100) using angle-resolved photoemission fine-structure spectroscopy*; Phys. Rev. B **48** (1993) 4760-4766

- [83] V. Fritzsche, S. Bao, Ph. Hofmann, M. Polcik, K.-M. Schindler, A.M. Bradshaw, R. Davis, D.P. Woodruff; *The adsorption of pyridine on Ni(111) determined by low-energy photoelectron diffraction*; Surf. Sci. **319** (1994) L1-L6
- [84] S. Bao, K.-M. Schindler, Ph. Hofmann, V. Fritzsche, A.M. Bradshaw, D.P. Woodruff; *The local adsorption structure of acetylene on Cu(111)*; Surf. Sci. **291** (1993) 295-308
- [85] K. Hermann, M. Witko; *Geometry and binding of acetylene on Cu(111): ab initio cluster studies*; Surf. Sci. **337** (1995) 205-214
- [86] D.I. Sayago, J.T. Hoeft, M. Polcik, M. Kittel, R.L. Toomes, J. Robinson, D.P. Woodruff, M. Pascal, C.L.A. Lamont, G. Nisbet; *Bond lengths and bond strengths in weak and strong chemisorption: N₂, CO, and CO/H on nickel surfaces*; Phys. Rev. Lett. **90**, 11 (2003) 116104-1, 116104-4
- [87] A.L. Linsebigler, G. Lu, J.T. Yates, Jr.; *Photocatalysis on TiO₂ Surfaces: Principles, Mechanisms, and Selected Results*; Chem. Rev. **95** (1995) 735-758
- [88] A. Mills, S. Le Hunte; *An overview of semiconductor photocatalysis*; J. of Photochemistry and Photobiology A: Chemistry **108** (1997) 1-35
- [89] O. Legrini, E. Oliveros, A.M. Braun; *Photochemical Processes for Water Treatment*; Chem. Rev. **93** (1993) 671-698
- [90] D.M. Blake; *Bibliography of Work on the Heterogeneous Photocatalytic Removal of Hazardous Compounds from Water and Air*; National Renewable Energy Laboratory NREL/TP-570-26797 (1994)
- [91] S. Klosek, D. Rafty; *Visible Light Driven V-Doped TiO₂ Photocatalyst and Its Photooxidation of Ethanol*; J. Phys. Chem. B **105** (2001) 2815-2819
- [92] W. Xiaohong, J. Zhaojun, L. Huiling, X. Shingang, H. Xinguo; *Photo-catalytic activity of titanium dioxide thin films prepared by micro-plasma oxidation method*; Thin Solid Films **441** (2003) 130-134
- [93] K.P. Khn, I.F. Chaberny, K. Massholder, M. Stickler, V.W. Benz, H.G. Sonntag, L. Erdinge; *Disinfection of surfaces by photocatalytic oxidation with titanium dioxide and UVA light*; Chemosphere **53** (2003) 71-77
- [94] <<http://www.epa.gov>>
- [95] <<http://www.eea.eu.int>>
- [96] G. Lu, A. Linsebigler, J.T. Yates, Jr.; *Photoxidation of CH₃Cl on TiO₂(110): A Mechanism Not Involving H₂O*; J. Phys. Chem. **99** (1995) 7626-7631

- [97] H. Onishi, T. Aruga, C. Egawa, Y. Iwasawa; *Catalytic Reactions on a Metal Oxide Single Crystal: Switchover of the Reaction Paths in Formic Acid Decomposition on TiO₂(110)*; Surf. Sci. **193** (1995) 33-46
- [98] H. Onishi, T. Aruga, Y. Iwasawa; *Adsorption of CH₃OH, HCOOH and SO₂ on TiO₂(110) and stepped TiO₂(441) surfaces*; J. Am. Chem. Soc. **115** (1993) 10460-10461
- [99] H. Onishi, T. Aruga, Y. Iwasawa; *Switchover of Reaction Paths in the Catalytic Decomposition of Formic Acid on TiO₂(110) surfaces*; J. Catal. **146** (1994) 557-567
- [100] H. Onishi, Y. Iwasawa; *STM-imaging of formate intermediates adsorbed on a TiO₂(110) surface*; Chem. Phys. Lett. **226** (1994) 111-114
- [101] H. Onishi, Y. Iwasawa; *STM observation of surface reactions on a metal oxide*; Surf. Sci. **357-358** (1996) 773-776
- [102] M. A. Henderson; *Complexity in the Decomposition of Formic Acid on the TiO₂(110) surface*; J. Phys. Chem. **101** (1997) 221-229
- [103] L.Q. Wang, K.F. Ferris, A.N. Shultz, D.R. Baer, M.H. Engelhard; *Interactions of HCOOH with stoichiometric and defective TiO₂(110) surfaces*; Surf. Sci. **380** (1997) 352-364
- [104] S.A. Chambers, S. Thevuthasan, Y.J. kim, G.S. Herman, Z. Wang, E. Tober, R. Ynzunza, J. Morais, C.H.F. Peden, K. Ferris, C.S. Fadley; *Chemisorption geometry of formate on TiO₂(110) by photoelectron diffraction*; Chem. Phys. Lett. **267** (1997) 51-57
- [105] S. Thevuthasan, G.S. Herman, Y.J. kim, S.A. Chambers, C.H.F. Peden, Z. Wang, R. Ynzunza, E.D. Tober J. Morais, C.S. Fadley; *The structure of formate on TiO₂(110) by scanned-energy and scanned-angle photoelectron diffraction*; Surf. Sci. **401** (1998) 261-268
- [106] S.P. Bates, G. Kresse, M.J. Gillan; *The adsorption and dissociation of ROH molecules on TiO₂(110)*; Surf. Sci. **409** (1998) 336-349
- [107] S.A. Chambers, M.A. Henderson, Y.J. Kim, S. Thevuthasan; *Chemisorption geometry, vibrational spectra, and thermal desorption of formic acid on TiO₂(110)*; Surf. Rev. and Lett. **5**,1 (1998) 381-385
- [108] Y. Iwasawa, H. Onishi, K.I. Fukui, S. Suzuki, T. Sasaki; *The selective adsorption and kinetic behaviour of molecules on TiO₂(110) observed by STM and NC-AF*; Faraday Discuss. **114** (1999) 259-266

- [109] B.E. Hayden, A. King, M.A. Newton; *Fourier Transform Reflection-Absorption IR spectroscopy Study of Formate Adsorption on TiO₂(110)*; J. Phys. Chem. B **103** (1999) 203-208
- [110] R.A. Bennet, P. Stone, R.D. Smiglak, M. Bowker; *Formic acid adsorption and decomposition on non-stoichiometric TiO₂(110)*; Surf. Sci. **454-456** (2000) 390-395
- [111] Z. Chang, G. Thornton; *Reactivity of thin-film TiO₂(110)*; Surf. Sci. **462** (2000) 68-76
- [112] P. Käckell, K. Terakura; *Dissociative adsorption of formic acid and diffusion of formate on the TiO₂(110) surface: the role of hydrogen*; Surf. Sci. **461** (2000) 191-198
- [113] P. Käckell, K. Terakura; *First principle analysis of the dissociative adsorption of formic acid on rutile TiO₂(110)*; Appl. Surf. Sci. **166** (2000) 370-375
- [114] L. Kieu, P. Boyd, H. Idriss; *Modelling of the adsorption of formic acid and formaldehyde over rutile TiO₂(110) and TiO₂(011) clusters*; J. of Molec. Catal. A: Chemical **176** (2001) 117-125
- [115] A. Gutierrez-Sosa, P. Martinez-Escalano, H. Raza, R. Lindsay, P.L. Wincott, G. Thornton; *Orientation of carboxylates on TiO₂(110)*; Surf. Sci. **471** (2001) 163-169
- [116] Y. Iwasawa, H. Onishi, K.I. Fukui; *In situ STM study of surface catalytic reactions on TiO₂(110) relevant to catalyst design*; Topics in Catalysis **14**, 1-4 (2001) 163-172
- [117] L-F. Liao, W.C. Wu, C.Y. Chen, J.L. Lin; *Photoxidation of Formic Acid vs Formate and Ethanol vs Ethoxy on TiO₂ and Effect of Adsorbed Water on the Rates of Formate and Formic Acid Photoxidation*; J. Phys. Chem. B **105** (2001) 7678-7685
- [118] M. Bowker, P. Stone, R. Bennet, N. Perkins; *Formic acid adsorption and decomposition on TiO₂(110) and on Pd/TiO₂(110) model catalyst*; Surf. Sci. **511** (2002) 435-448
- [119] D.S. Muggli, M.J. Backes; *Two Active Sites for Photocatalytic Oxidation of Formic Acid on TiO₂: Effects of H₂O and Temperature*; J. of Catal. **209** (2002) 105-113
- [120] H. Onishi, A. Sasashara, H. Uetsuka, T.A. Ishibashi; *Molecule-dependent topography determined by noncontact atomic force microscopy: carboxylates on TiO₂(110)*; Appl. Surf. Sci. **188** (2002) 257-264
- [121] R. Patel, Q. Guo, I. Cocks, E.M. Williams, E. Roman, J.L. de Segovia; *The defective nature of the TiO₂(110)(1x2)surface*; J. Vac. Sci. Technol. A **15**(5) (1997) 1-4
- [122] Various authors; *The Chemical Physics of Solid Surfaces, vol 9, Oxide Surfaces*; Ed. D.P. Woodruff (2001) Elsevier, Amsterdam

- [123] P.W. Tasker; *The stability of ionic crystal surfaces*; J. Phys. C: Solid State Phys. **12** (1979) 4977-4984
- [124] J.P. LaFemina; Crit. Rev. Surf. Chem. **3** (1994) 297-386
- [125] B. Hird, R.A. Armstrong; *Ion scattering measurements of rutile $TiO_2(110)$ -(1x1) surface relaxation*; Surf. Sci. **385** (1997) L1023-L1028
- [126] G. Charlton, P.B. Howes, C.L. Nicklin, P. Steadman, J.S.G. Taylor, C.A. Muryn, S.P. Harte, J. Mercer, R. McGrath, D. Norman, T.S. Turner, G. Thornton; *Relaxation of $TiO_2(110)$ -(1x1) Using Surface X-Ray Diffraction*; Phys. Rev. Lett. **78**, 3 (1997) 495-498
- [127] B. Hird, R.A. Armstrong; *Surface relaxation of rutile $TiO_2(110)$ -(1x1) from ion shadowing/blocking measurements*; Surf. Sci. **420** (1999) L131-L137
- [128] A. Verdini, M. Sambi, F. Bruno, D. Cvetko, M. Della Negra, R. Gotter, L. Floreano, A. Morgante, G.A. Rizzi, G. Granozzi; *Determination of $TiO_2(110)$ surface relaxation by variable polarization photoelectron diffraction*; Surf. Rev. and Lett. **6**, 6 (1999) 1201-1206
- [129] E. Asari, T. Suzuki, H. Kawanowa, J. Ahn, W. Hayami, T. Aizawa, R. Souda; *$TiO_2(110)$ - p (1x1) surface structure analyzed by impact-collision ion-scattering spectroscopy*; Phys. Rev. B **61**, 8 (2000) 5679-5682
- [130] R. Lindsay, C. Thornton, A. Wander, N.M. harrison, A. Ernst; To be published
- [131] D. Vogtenhuber, R. Podloucky, A. Neckel, S.G. Steinemann, A.J. Freeman; *Electronic structure and relaxed geometry of the TiO_2 rutile (110) surface*; Phys. Rev. B **49**, 3 (1994) 2099-2103
- [132] M. Ramamoorthy, D. Vanderbilt; *First-principles calculations of the energetics of stoichiometric TiO_2 surfaces*; Phys. Rev. B **49**, 23 (1994) 16721-16727
- [133] P.J.D. Lindan, N.M. Harrison, M.J. Gillan, J.A. White; *First-principles spin-polarized calculations on the reduced and reconstructed TiO_2 (110) surface*; Phys. Rev. B **55**, 23 (1997) 15919-15927
- [134] N.M. Harrison, X.G. Wang, J. Muscat, M. Scheffler; *The influence of soft vibrational modes on our understanding of oxide surface structure*; Faraday Discuss., Chem. Soc.**114** (1999) 305-312
- [135] P. Reinhardt, B.A. Hess; *Electronic and geometrical structure of rutile surfaces*; Phys. Rev. B. **50** (1994) 12015-12024
- [136] S.P. Bates, M.J. Gillan, G. Kresse; *A systematic study of the surface energetics and structure of TiO_2 by first principles calculations*; Surf. Sci. **385** (1997) 386-394

- [137] M. Li, W. Hebenstreit, U. Diebold, A.M. Tyryshkin, M.K. Bowman, G.G. Dunham, M.A. Henderson; *The influence of the bulk reduction state on the surface structure and morphology of rutile TiO_2 (110) single crystals*; J. Phys. Chem. B **104** (2000) 4944-4950
- [138] R. Schaub, P. Thostrup, N. Lopez, E. Laegsgaard, I. Stensgaard, J.K. Norskov, F. Besenbacher; *Oxygen vacancies as active sites for water dissociation on rutile TiO_2 (110)*; Phys. Rev. Lett. **87**, 26 (2001) 266104-1,266104-4
- [139] W. Gpel, J.A. Anderson, D. Frankel, M. Jaehnig, K. Phillips, J.A. Schfer, G. Rocker; *Surface Defects of TiO_2 (110): A combined XPS, XAES and ELS study*; Surf. Sci. **139** (1984) 333-346
- [140] M.A. Henderson; *Evidence for bicarbonate formation on vacuum annealed TiO_2 (110) resulting from a precursor-mediated interaction between CO_2 and H_2O* ; Surf. Sci. **400** (1998) 203-219
- [141] K.I. Fukui, H. Onishi, Y. Iwasawa; *Atom-resolved image of the TiO_2 (110) surface by noncontact atomic force microscopy*; Phys. Rev. Lett. **79**, 21 (1997) 4202-4205
- [142] M.L. Knotek, P.J. Feibelman; *Stability of ionically bonded surfaces in ionizing environments*; Surf. Sci. **90** (1979) 78-90
- [143] L.Q. Wang, D.R. Baer, M.H. Engelhard; *Creation of variable concentrations of defects on TiO_2 (110) using low-density electron beams*; Surf. Sci. **320** (1994) 295-306
- [144] L.Q. Wang, D.R. Baer, M.H. Engelhard, A.N. Schultz; *The adsorption of liquid and vapor water on TiO_2 surface: the role of defects*; Surf. Sci. **344** (1995) 237-250
- [145] U. Diebold; *The surface science of titanium dioxide*; Surf. Sci. Rep. **48** (2003) 53-229
- [146] M.A. Henderson, W.S. Epling, C.L. Perkins, C.H.F. Peden, U. Diebold; *Interaction of molecular oxygen with the vacuum-annealed TiO_2 (110) surface: molecular and dissociative channels*; J. Phys. Chem. B **103** (1999) 5328-5337
- [147] J. Stöhr, D. Outka, R.J. Madix, U. Döbler; *Evidence for a novel chemisorption bond: formate (HCO_2) on $Cu(100)$* ; Phys. Rev. Lett. **54** (1985) 1256-1259
- [148] D.P. Woodruff, C.F. McConville, A.L.D. Kilcoyne, Th. Linder, J. Somers, M. Surman, G. Paolucci, A.M. Bradshaw; *The structure of the formate species on copper surfaces: new photoelectron diffraction and SEXAFS data reassessed*; Surf. Sci. **201** (1988) 228-244
- [149] M. Sambi, G. Granozzi, M. Casarin, G.A. Rizzi, A. Vittadini, L.S. Caputi, G. Chiarello; *Surface carboxylate species on $Cu(100)$ studied by angle-scanned photoelectron diffraction and LCAO-LDF calculations*; Surf. Sci. **315** (1994) 309-322

- [150] U. Hergenhahn, E.E. Rennie, O. Kugeler, S. Marburger, T. Lischke, I. Powis, G. Garcia; *Photoionization circular dichroism in core level ionization of randomly oriented pure enantiomers of the chiral molecule camphor*; J. Chem. Phys. **120** (2004) 4553-4556
- [151] L.L. Atanasoska, J.C. Buchholz and G.A. Somorjai; *Low-energy electron diffraction study of the surface structures of adsorbed amino acid monolayers and ordered films deposited on copper crystal surfaces*; Surf. Sci. **72** (1978) 189-207
- [152] R.J. Colton, J.S. Murday, J.R. Wyatt, J.J. De Corpo; *Combined XPS and SIMS study of amino acid overlayers*; Surf. Sci. **84** (1979) 235-248
- [153] J.S. Suh, M. Moskovits; *Surface-enhanced Raman spectroscopy of amino acids and nucleotide bases adsorbed on Silver*; J. Am. Chem. Soc. **108** (1986) 4711-4718
- [154] A. Ihs, B. Liedberg, K. Udval, C. Törnkvist, P. Bodoö, I. Lündstrom; *Infrared and photoelectron spectroscopy of amino acids on Cooper: glycine, L-alanine and β -alanine*; Journal of Colloid and Interface Science **140**, 1 (1990) 192-206
- [155] J. Williams, S. Haq, R. Raval; *The bonding and orientation of the amino acid L-alanine on Cu110 determined by RAIRS*; Surf. Sci. **368** (1996) 303-309
- [156] Xueying Zhao, R.G. Zhao, W.S. Yang; *Adsorption of alanine on Cu(001) studied by scanning tunneling microscopy*; Surf. Sci. **442** (1999) L995-L1000
- [157] R. Raval; *Assembling molecular guidance systems for heterogeneous enantioselective catalysis*; CATTECH **5**, 1 (2001) 12-28
- [158] Chiksahi Egawa, Hidekazu Iwai, Masaki Kabuyota, Shoichi Oki; *STM study of DL-alanine array structure on Cu(001)*; Surf. Sci. **532-535** (2003) 233-236
- [159] S. Barlow, R. Raval; *Complex organic molecules at metal surfaces: bonding, organisation and chirality*; Surf. Sci. Rep. **50** (2003) 201-341
- [160] D.T. Clark, J. Peeling, L. Colling; *An experimental and theoretical investigation of the core level spectra of a series of amino acids, dipeptides and polypeptides*; Biochim. Biophys. Acta - Protein structure **453**, 2 (1976) 533-545
- [161] P. Löfgren, A. Krozer, J. Lausmaa, B. Kasemo; *Glycine on Pt(111): a TDS and XPS study*; Surf. Sci. **370**, 1 (1997) 277-292
- [162] N.A. Booth, D.P. Woodruff, O. Schaff, T. Gießel, R. Lindsay, P. Baumgärtel, A.M. Bradshaw; *Determination of the local structure of glycine adsorbed on Cu(110)*; Surf. Sci. **397** (1998) 258-269
- [163] J.-H. Kang, R.L. Toomes, M. Polcik, M. Kittel, J.-T. Hoeft, V. Efstathiou, D.P. Woodruff, A.M. Bradshaw; *Structural investigation of glycine on Cu(100) and comparison to glycine on Cu(110)*; J. Chem. Phys. **118**, 13 (2003) 6059-6071

- [164] M. Nyberg, M. Odelius, A. Nilsson, L.G.M. Pettersson; *Hydrogen bonding between adsorbed deprotonated glycine molecules on Cu(110)*; J. Chem. Phys. **119**, 23 (2003) 12577-12585
- [165] B. Ritchie; *Theory of the angular distribution of photoelectrons ejected from optically active molecules and molecular negative ions*; Phys. Rev. A **13**, 4 (1975) 1411-1415
- [166] N.A. Cherepkov; *Circular dichroism of molecules in the continuous adsorption region*; Chem. Phys. Lett. **87**, 4 (1982) 344-348
- [167] I. Powis; *Photoelectron spectroscopy and circular dichroisms in chiral biomolecules: L-alanine*; J. Phys. Chem. A **104** (2000) 878-882
- [168] R.L. Dubs, S.N. Dixit, V. Mckoy; *Circular dichroisms in photoelectron angular distributions from oriented linear molecules*; Phys. Rev. Lett. **54**, 12 (1985) 1249-1251
- [169] G. Schönhense; *Circular dichroisms and spin polarization in photoemission from adsorbates and non-magnetic solids*; Phys. Scripta **T31** (1990) 255-275
- [170] C. Westphal, J. Bansmann, M. Getzlaff, G. Schönhense; *Circular dichroism in the angular distribution of photoelectrons from oriented CO molecules*; Phys. Scripta **T31** (1990) 255-275
- [171] N. Chandra; *Circular dichroism in photoionization of oriented nonlinear molecules*; Phys. Rev. A **39**, 4 (1989) 2256-2259
- [172] H. Daimon, T. Nakatani, S. Imada, S. Suga, Y. Kagoshima, T. Miyahara; *Strong circular dichroism in photoelectron diffraction from nonchiral nonmagnetic material-Direct observation of rotational motion of electrons*; Jpn. J. Appl. Phys. **32** (1993) L1480-L1483
- [173] C. Westphal, A.P. Kaduwela, C.S. Fadley, M.A. Van Hove; *Photoelectron-diffraction effects and circular dichroism in core-level photoemission*; Phys. Rev. B **50**, 9 (1994) 6203-6208
- [174] G.A. Attard, D. Watson, E.A. Seddon, S.M. Cornelius, E. Herrero, J. Feliu; *Photoemission studies of chiral metal surfaces using circularly polarized synchrotron radiation*; Phys. Rev. B **64** (2001) 115408-1, 115408-6
- [175] I. Stensgaard; *Adsorption of di-L alanine on Cu(110) investigated with scanning tunneling microscopy*; Surf. Sci. **545** (2003) L747-L752
- [176] G. Ertl; *Heterogeneous catalysis on atomic scale*; Journal of Mol. Catal. A: Chemical **182-183** (2002) 5-16