

Bibliography

- [And05] M. Andersson. private communication (2005).
- [Ani74] S.I. Anisimov, B.L. Kapeliovich, and T.L. Perel'man. *Electron emission from metal surfaces exposed to ultrashort laser pulses*. Sov. Phys. JETP **39**, (1974) 375.
- [Ant80] P.R. Antoniewicz. *Model for electron- and photon-stimulated desorption*. Phys. Rev. B **21**, (1980) 3811.
- [Ash01] N.W. Ashcroft and N.D. Mermin. *Festkörperphysik*. Oldenbourg, München (2001).
- [Atk87] P.W. Atkins. *Physikalische Chemie*. Wiley VCH (1987).
- [Avo89] P. Avouris and R.E. Walkup. *Fundamental Mechanisms of Desorption and Fragmentation Induced by Electronic Transitions at Surfaces*. Annu. Rev. Phys. Chem. **40**, (1989) 173.
- [Bac05] E.H.G. Backus, A. Eichler, A.W. Kleyn, and M. Bonn. *Real-Time Observation of Molecular Motion on a Surface*. Science **310**, (2005) 1790.
- [Bas82] J Bass. *Electrical Resistivity, Kondo and Spin Fluctuation Systems, Spin Glasses and Thermopower*, volume III/15a of *Landolt-Börnstein*, page 70. Springer, Berlin (1982).
- [Bjo75] G.C. Bjorklund. *Effects of Focusing on Third-Order Nonlinear Processes in Isotropic Media*. IEEE J. Quantum Electronics **11**, (1975) 287.
- [Bon99] M. Bonn, S. Funk, Ch. Hess, D.N. Denzler, C. Stampfl, M. Scheffler, M. Wolf, and G. Ertl. *Phonon- Versus Electron-Mediated Desorption and Oxidation of CO on Ru(0001)*. Science **285**, (1999) 1042.
- [Bon00a] M. Bonn, D.N. Denzler, S. Funk, M. Wolf, S.S. Wellershof, and J. Hohlfeld. *Ultrafast electron dynamics at metal surfaces: Competition between electron-phonon coupling and hot-electron transport*. Phys. Rev. B **61**, (2000) 1101.
- [Bon00b] M. Bonn, Ch. Hess, S. Funk, J. Miners, B.N.J. Persson, M. Wolf, and G. Ertl. *Femtosecond Surface Vibrational Spectroscopy of CO on Ru(001) during Desorption*. Phys. Rev. Lett. **84**, (2000) 4653.
- [Bon01] M. Bonn, C. Hess, and M. Wolf. *The dynamics of vibrational excitation on surfaces: CO on Ru(001)*. J. Chem. Phys. **115**, (2001) 7725.

Bibliography

- [Bon04] M. Bonn, C. Hess, W.G. Roeterdink, H. Ueba, and M. Wolf. *Dephasing of vibrationally excited molecules at surfaces: CO/Ru(001)*. Chem. Phys. Lett. **388**, (2004) 269.
- [Bor27] M. Born and R. Oppenheimer. *Zur Quantentheorie der Molekeln*. Ann. Phys. **84**, (1927) 457.
- [Bra95] M. Brandbyge, P. Hedegard, T.F. Heinz, J.A. Misewich, and D.M. Newns. *Electronically driven adsorbate excitation mechanism in femtosecond-pulse laser desorption*. Phys. Rev. B **52**, (1995) 6042.
- [Bre76] W. Brenig and K. Schönhammer. *A "Hydrodynamic" Theory of Surface Reaction Rates*. Z. Physik B **24**, (1976) 91.
- [Bri99] G.P. Brivio and M.I. Trioni. *The adiabatic molecule-metal surface interaction: Theoretical approaches*. Rev. Mod. Phys. **71**, (1999) 1999.
- [Bud91] F. Budde, T.F. Heinz, M.M.T. Loy, J.A. Misewich, F. de Rougemont, and H. Zacharias. *Femtosecond time-resolved measurement of desorption*. Phys. Rev. Lett. **66**, (1991) 3024.
- [Bud93] F. Budde, T.F. Heinz, A. Kalamarides, M.M.T. Loy, and J.A. Misewich. *Vibrational distributions in desorption induced by femtosecond laser pulses: coupling of adsorbate vibration to substrate electronic excitation*. Surf. Sci **283**, (1993) 143.
- [Cha90] H.C. Chang and G.E. Ewing. *Vibrational Energy Transfer and Population Inversion in CO Overlayers on NaCl(100)*. J. Phys. Chem. **94**, (1990) 7635.
- [Cho87] M.Y. Chou and J.R. Chelikowsky. *First-principles study of hydrogen adsorption on Ru(0001): Possible occupation of subsurface sites*. Phys. Rev. Lett. **59**, (1987) 1737.
- [Cho89] M.Y. Chou and J.R. Chelikowsky. *Theoretical study of hydrogen adsorption on Ru(0001): Possible surface and subsurface occupation sites*. Phys. Rev. B **39**, (1989) 5623.
- [Cho03] I. Chorkendorff and J.W. Niemantsverdriet. *Concepts of Modern Catalysis and Kinetics*. Wiley VCH, Weinheim (2003).
- [Chr91] K. Christmann. *Introduction to Surface Physical Chemistry*. Steinkopff, Darmstadt (1991).
- [Com85] G. Comsa and R. David. *Dynamical Parameters of Desorbing Molecules*. Surf. Sci. Rep. **5**, (1985) 145.
- [Cow78] J.P. Cowin, D.J. Auerbach, C. Becker, and L. Wharton. *Measurement of fast desorption kinetics of D₂, from tungsten by laser induced thermal desorption*. Surf. Sci. **78**, (1978) 545.
- [d'A73] E.G. d'Agliano, W. Schaich, P. Kumar, and H. Suhl. *Reaction Kinetics at Solid Surfaces*. In B. Lundquist and S. Lundquist (Editors), *Nobel Symposia: Collective Properties of Physical Systems*, volume 24. Academic Press, New York - London (1973).

- [d'A75] E.G. d'Agliano, P. Kumar, W. Schaich, and H. Suhl. *Brownian motion model of the interaction between chemical species and metallic electrons: Bootstrap derivation and parameter evaluation*. Phys. Rev. B **11**, (1975) 2122.
- [Dah98] S. Dahl, P.A. Taylor, E. Törnquist, and I. Chorkendorff. *The Synthesis of Ammonia over a Ruthenium Single Crystal*. J. Catal. **178**, (1998) 679.
- [Dah99] S. Dahl, A. Logadottir, R.C. Egeberg, J.H. Larsen, I. Chorkendorff, E. Törnquist, and J.K. Nørskov. *Role of Steps in N₂ Activation on Ru(0001)*. Phys. Rev. Lett. **83**, (1999) 1814.
- [Dah00a] S. Dahl, J. Sehested, C.J.H. Jacobsen, E. Törnquist, and I. Chorkendorff. *Surface science based microkinetic analysis of ammonia synthesis over ruthenium catalysts*. J. Catal. **192**, (2000) 391.
- [Dah00b] S. Dahl, E. Törnqvist, and I. Chorkendorff. *Dissociative Adsorption of N₂ on Ru(0001): A Surface Reaction Totally Dominated by Steps*. J. Catal. **192**, (2000) 381.
- [Dan93] R. Danielius, A. Piskarskas, A. Stabinis, G.P. Banfi, P. Di Trapani, and R. Righini. *Travelling-wave parametric generation of widely tunable, highly coherent femtosecond light pulses*. J. Opt. Soc. Am. B **10**, (1993) 2222.
- [Dar95] G.R. Darling and S. Holloway. *The dissociation of diatomic molecules at surfaces*. Rep. Prog. Phys. **58**, (1995) 1595.
- [Daw72] P.T. Dawson and Y.K. Peng. *On the λ -state of nitrogen on tungsten surfaces*. Surf. Sci. **33**, (1972) 565.
- [Del95] S. Deliwala, R.J. Finlay, J.R. Goldmann, T.H. Her, W.D. Mieber, and E. Mazur. *Surface femtochemistry of O₂ and CO on Pt(111)*. Chem. Phys. Lett. **242**, (1995) 617.
- [Dem98] W. Demtröder. *Laser Spectroscopy*. Springer, Berlin, 2. corr. edition (1998).
- [Den99] D.N. Denzler. *Untersuchungen zur Ultrakurzzeitdynamik photostimulierter Oberflächenreaktionen und der Energierelaxation in Metallen*. Diplomarbeit. Freie Universität Berlin, Fachbereich Physik (1999).
- [Den03a] D.N. Denzler. *Zur ultraschnellen Reaktionsdynamik von Wasserstoff und Grenzflächenstruktur von Wasser auf der Ru(001)-Oberfläche*. Ph.D. thesis, Freie Universität Berlin, Fachbereich Physik (2003).
- [Den03b] D.N. Denzler, C. Frischkorn, C. Hess, M. Wolf, and G. Ertl. *Electronic Excitation and Dynamic Promotion of a Surface Reaction*. Phys. Rev. Lett. **91**, (2003) 226102.
- [Den04] D.N. Denzler, C. Frischkorn, M. Wolf, and G. Ertl. *Surface Femtochemistry: Associative Desorption of Hydrogen from Ru(001) Induced by Electronic Excitations*. J. Phys. Chem. B **108**, (2004) 14503.
- [Día06a] C. Díaz, J.K. Vincent, G.P. Krishnamohan, R.A. Olsen, G.J. Kroes, K. Honkala, and J.K. Nørskov. *Multidimensional Effects on Dissociation of N₂ on Ru(0001)*. Phys. Rev. Lett. **96**, (2006) 096102.

Bibliography

- [Día06b] C. Díaz, J.K. Vincent, G.P. Krishnamohan, R.A. Olsen, G.J. Kroes, K. Honkala, and J.K. Nørskov. *Reactive and nonreactive scattering of N_2 from $Ru(0001)$: A six-dimensional adiabatic study*. J. Chem. Phys. **125**, (2006) 114706.
- [Die00a] L. Diekhöner. *Dynamics of High Barrier Gas-Surface Reactions studied by Laser Assisted Associative Desorption*. Ph.D. thesis, Fysisk Institut, Syddansk Universitet - Odense Universitet (2000).
- [Die00b] L. Diekhöner, H. Mortensen, A. Baurichter, A.C. Luntz, and B. Hammer. *Dynamics of High-Barrier Surface Reactions: Laser-Assisted Associative Desorption of N_2 from $Ru(0001)$* . Phys. Rev. Lett **84**, (2000) 4906.
- [Die01] L. Diekhöner, H. Mortensen, A. Baurichter, and A.C. Luntz. *Laser assisted associative desorption of N_2 and CO from $Ru(0001)$* . J. Chem. Phys. **115**, (2001) 3356.
- [Die02] L. Diekhöner, L. Hornekær, H. Mortensen, E. Jensen, A. Baurichter, V.V. Petrunin, and A.C. Luntz. *Indirect evidence for strong nonadiabatic coupling in N_2 associative desorption from and dissociative adsorption on $Ru(0001)$* . J. Chem. Phys. **117**, (2002) 5018.
- [Diñ00] W.A. Diño, H. Kasai, and A. Okiji. *Orientational effects in dissociative adsorption/associative desorption dynamics of $H_2(D_2)$ on Cu and Pd* . Prog. Surf. Sci. **63**, (2000) 63.
- [Eic99] A. Eichler, J. Hafner, A. Groß, and M. Scheffler. *Trends in the chemical reactivity of surfaces studied by ab initio quantum-dynamics calculations*. Phys. Rev. B **59**, (1999) 13297.
- [Eva35] M.G. Evans and M. Polanyi. *Some applications of the transition state method to the calculation of reaction velocities, especially in solution*. Trans. Faraday Soc. **31**, (1935) 875.
- [Eyr31] H. Eyring and M. Polanyi. *Über einfache Gasreaktionen*. Z. Phys. Chem. Abt. B **12**, (1931) 279.
- [Eyr35] H. Eyring. *The activated complex and the absolute rate of chemical reactions*. Chem. Rev. **17**, (1935) 65.
- [Fan92a] W.S. Fann, R. Storz, H.W.K. Tom, and J. Bokor. *Direct measurement of nonequilibrium electron-energy distributions in subpicosecond laser-heated gold films*. Phys. Rev. L. **68**, (1992) 2834.
- [Fan92b] W.S. Fann, R. Storz, H.W.K. Tom, and J. Bokor. *Electron Thermalization in Gold*. Phys. Rev. B. **46**, (1992) 13596.
- [Fei94] P.J. Feibelman, J.E. Houston, H.L. Davis, and D.G. O'Neill. *Relaxation of the clean, Cu - and H -covered $Ru(0001)$ surface*. Surf. Sci. **302**, (1994) 81.
- [Feu80] P. Feulner and D. Menzel. *Simple ways to improve 'flash desorption' measurements from single crystal surfaces*. J. Vac. Sci. Tech. **17**, (1980) 662.

- [Feu85] P. Feulner and D. Menzel. *The adsorption of hydrogen on ruthenium (001): Adsorption states, dipole moments and kinetics of adsorption and desorption*. Surf. Sci. **154**, (1985) 465.
- [Fli97] T. Fließbach. *Elektrodynamik*. Spektrum Akademischer Verlag, Heidelberg (1997).
- [Fri06] C. Frischkorn and M. Wolf. *Femtochemistry at Metal Surfaces: Nonadiabatic Reaction Dynamics*. Chem. Rev. (in press).
- [Fun99] S. Funk. *Ultraschnelle Dynamik an Oberflächen: Desorption und Oxidation von CO auf Ruthenium induziert durch Femtosekunden-Laserpulse*. Ph.D. thesis, Freie Universität Berlin, Fachbereich Physik (1999).
- [Fun00] S. Funk, D.N. Denzler, C. Hess, M. Wolf, and G. Ertl. *Desorption of CO from Ru(001) induced by near-infrared femtosecond laser pulses*. J. Chem. Phys. **112**, (2000) 9888.
- [Ger87] R.B. Gerber. *Molecular Scattering from Surfaces*. Chem. Rev. **87**, (1987) 29.
- [Ger01] B. Gergen, H. Nienhaus, W.H. Weinberg, and E.W. McFarland. *Chemically Induced Electronic Excitations at Metal Surfaces*. Science **294**, (2001) 2521.
- [Gla41] S. Glasstone, K.J. Laidler, and H. Eyring. *The Theory of Rate Processes*. McGraw-Hill, New York-London (1941).
- [Goo92] L. Goodman and J. Philis. *Multiphoton Absorption Spectroscopy*. In D.L. Andrews (Editor), *Applied Laser Spectroscopy*, page 227. VCH, New York (1992).
- [Gre82] C.H. Greene and R.N. Zare. *Photofragment alignment and orientation*. Ann. Rev. Phys. Chem. **33**, (1982) 119.
- [Gre97] H. Greber. *Charge-transfer induced particle emission in gas surface reactions*. Surf. Sci. Rep. **28**, (1997) 1.
- [Gri81a] E.K. Grimmelmann, J.C. Tully, and E. Helfand. *Molecular dynamics of infrequent events: Thermal desorption of xenon from a platinum surface*. J. Chem. Phys. **74**, (1981) 5300.
- [Gri81b] G. Grimvall. *The Electron-Phonon Interaction in Metals*. In E.P. Wohlfarth (Editor), *Selected Topics in Solid State Physics*, volume XVI. North-Holland, Amsterdam (1981).
- [Gro95] R.H.M. Groeneveld, R. Sprik, and A. Lagendijk. *Femtosecond Spectroscopy of Electron-Electron and Electron-Phonon Energy Relaxation in Ag and Au*. Phys. Rev. B **51**, (1995) 11433.
- [Gro96a] A. Groß and M. Scheffler. *Influence of molecular vibrations on dissociative adsorption*. Chem. Phys. Lett. **256**, (1996) 417.
- [Gro96b] A. Groß and M. Scheffler. *Steering and ro-vibrational effects on dissociative adsorption and associative desorption of H₂/Pd(100)*. Prog. Surf. Sci. **53**, (1996) 187.

Bibliography

- [Gro98] A. Groß. *Reactions at surfaces studied by ab initio dynamics calculations*. Surf. Sci. Rep. **32**, (1998) 291.
- [Hab05] F. Haber and G. van Oordt. *Über die Bildung von Ammoniak aus den Elementen*. Z. Anorg. Chem. **44**, (1905) 341.
- [Hal90] D. Halstead and S. Holloway. *The influence of potential energy surface topologies on the dissociation of H₂*. J. Chem. Phys. **93**, (1990) 2859.
- [Hal95] J.B. Halpern, R. Dopheide, and H. Zacharias. *How a collision causes misalignment: alignment decay in acetylene 2¹*. J. Phys. Chem. **99**, (1995) 13611.
- [Ham00a] B. Hammer. *Adsorption, diffusion, and dissociation of NO, N and O on flat and stepped Ru(0001)*. Surf. Sci. **459**, (2000) 323.
- [Ham00b] B. Hammer and J.K. Nørskov. *Theoretical surface science and catalysis - calculations and concepts*. Advances in Catalysis **45**, (2000) 71.
- [Han90] M. Hand and J. Harris. *Recoil effects in surface dissociation*. J. Chem. Phys. **92**, (1990) 7610.
- [Has95] E. Hasselbrink. *State-resolved Probes of molecular Desorption Dynamics induced by short-lived electronic Excitations*. In H.-L. Dai, W. Ho (Editor), *Laser Spectroscopy and Photochemistry on Metal Surfaces*, page 685. World Scientific, Singapore (1995).
- [Hea95] M. Head-Gordon and J.C. Tully. *Molecular dynamics with electronic frictions*. J. Chem. Phys. **103**, (1995) 10137.
- [Hel84] B. Hellsing and M. Persson. *Electronic Damping of Atomic and Molecular Vibrations at Metal Surfaces*. Physica Scripta **29**, (1984) 360.
- [Her98] T.H. Her, R.J. Finlay, C. Wu, and E. Mazur. *Surface femtochemistry of CO/O₂/Pt(111): The importance of nonthermalized substrate electrons*. J. Chem. Phys. **108**, (1998) 8595.
- [Hes00a] Ch. Hess, M. Bonn, S. Funk, and M. Wolf. *Hot-band excitation of CO chemisorbed on Ru(001) studied with broadband-IR sum-frequency generation*. Chem. Phys. Lett. **325**, (2000) 139.
- [Hes00b] Ch. Hess, M. Wolf, and M. Bonn. *Direct Observation of Vibrational Energy Delocalization on Surfaces: CO on Ru(001)*. Phys. Rev. Lett. **85**, (2000) 4341.
- [Hes01] C. Hess. *Ultrafast reaction dynamics and vibrational spectroscopy at surfaces*. Ph.D. thesis, Freie Universität Berlin, Fachbereich Chemie (2001).
- [Hes02] Ch. Hess, M. Wolf, S. Roke, and M. Bonn. *Femtosecond time-resolved vibrational SFG spectroscopy of CO/Ru(001)*. Surf. Sci. **502-503**, (2002) 304.
- [Hof85] P. Hoffmann and D. Menzel. *Synchrotron radiation studies of hydrogen adsorption on Ru(001)*. Surf. Sci. **152**, (1985) 382.

- [Hof91] F.M. Hoffmann, M.D. Weisel, and C.H.F. Peden. *In-situ FT-IRAS study of the CO oxidation reaction over Ru(001): II. Coadsorption of carbon monoxide and oxygen.* Surf. Sci. **253**, (1991) 59.
- [Hoh98] J. Hohlfeld. *Ultrafast Electron-, Lattice, and Spin-Dynamics in Metals investigated by linear and non-linear optical Techniques.* Ph.D. thesis, Freie Universität Berlin, Fachbereich Physik (1998).
- [Hol91] S. Holloway and J.K. Nørskov. *Bonding at Surfaces.* Liverpool University Press, Liverpool (1991).
- [Hrb85] J. Hrbek. *Carbonaceous overlayers on Ru(001).* J. Vac. Sci. Techn. A. **4**, (1985) 86.
- [Hun87] J.H. Hunt, P. Guyot-Sionnest, and Y.R. Shen. *Observation of C-H stretch vibrations of monolayers of molecules optical sum-frequency generation.* Chem. Phys. L. **133**, (1987) 189.
- [Jac86] D.C. Jacobs and R.N. Zare. *Reduction of 1+1 resonance enhanced MPI spectra to population and alignment factors.* J. Chem. Phys. **10**, (1986) 5457.
- [Jac00] C.J.H. Jacobsen. *Novel class of ammonia synthesis catalysts.* Chem. Comm. **12**, (2000) 1057.
- [Jam83] W. Jamroz and B.P. Stoicheff. *Generation of tunable coherent Vacuum-Ultraviolet Radiation.* In E. Wolf (Editor), *Progress in Optics XX*, page 327. North Holland, Amsterdam (1983).
- [Kag57] M.I. Kaganov, I.M. Lifshitz, and L.V. Tanatarov. *Relaxation between Electrons and the Crystalline Lattice.* Sov. Phys. JETP **4**, (1957) 173.
- [Kan98] A.P. Kanavin, I.V. Smetanin, V.A. Isakov, Y.V. Afanasiev, B.N. Chichkov, B. Wellegehausen, S. Nolte, C. Momma, and A. Tünnermann. *Heat transport in metals irradiated by ultrashort laser pulses.* Phys. Rev. B **57**, (1998) 14698.
- [Kao93a] F.-J. Kao, D.G. Busch, D. Cohen, D. Gomes da Costa, and W. Ho. *Femtosecond laser desorption of molecularly adsorbed oxygen from Pt(111).* Phys. Rev. Lett. **71**, (1993) 2094.
- [Kao93b] F.-J. Kao, D.G. Busch, D. Gomes da Costa, and W. Ho. *Femtosecond versus nanosecond surface photochemistry: O₂+CO on Pt(111) at 80 K.* Phys. Rev. Lett. **70**, (1993) 4098.
- [Kin78] D.A. King. *Kinetics of Adsorption, Desorption, and Migration at Single-Crystal Metal Surfaces.* CRC Crit. Rev. Solid State Mater. Sci. **7**, (1978) 167.
- [Kin98] J.T. Kindt, J.C. Tully, M. Head-Gordon, and M.A. Gomez. *Electron-hole pair contributions to scattering, sticking, and surface diffusion: CO on Cu(100).* J. Chem. Phys. **109**, (1998) 3629.
- [Kit96] C. Kittel. *Introduction to Solid State Physics.* John Wiley & Sons, New York (1996).

Bibliography

- [Kne99] S. Kneitz, J. Gemeinhardt, and H.-P. Steinrück. *A molecular beam study of the adsorption dynamics of CO on Ru(0001), Cu(111) and a pseudomorphic CU monolayer on Ru(0001)*. Surf. Sci. **440**, (1999) 307.
- [Koe96] W. Koechner. *Solid-State Laser Engineering*. Springer, Berlin, 3. edition (1996).
- [Kol94] K.W. Kolasinski, W. Nessler, A. de Meijere, and E. Hasselbrink. *Hydrogen adsorption on and desorption from Si: Considerations on the applicability of detailed balance*. Phys. Rev. Lett. **72**, (1994) 1356.
- [Kol02] K.W. Kolasinski. *Surface Science - Foundations of Catalysis and Nanoscience*. Wiley (2002).
- [Kos92] K.L. Kostov, H. Rauscher, and D. Menzel. *Adsorption of CO on Oxygen-covered Ru(001)*. Surf. Sci. **278**, (1992) 62.
- [Kov69] I. Kovács. *Rotational Structure in the spectra of Diatomic Molecules*. Adam Hilger LTD, London (1969).
- [Kra40] H.A. Kramers. *Brownian Motion in Field of Force and the Diffusion Model of Chemical Reactions*. Physica **7**, (1940) 284.
- [Lam77] J.D. Lambert. *Vibrational and Rotational Relaxation in Gases*. Clarendon, Oxford (1977).
- [Lau86] L.L. Lauderback and W.N. Delgass. *The structure and mobility of carbon on Ru(001)*. Surf. Sci. **172**, (1986) 715.
- [Lau87] L.L. Lauderback and W.N. Delgass. *CO Dissociation and C-D Interaction on Ru(001)*. J. Catalysis **105**, (1987) 55.
- [Len32] J.E. Lennard-Jones. *Processes of adsorption and diffusion on solid surfaces*. Trans. Faraday Soc. **28**, (1932) 333.
- [Lin87a] M. Lindroos, H. Pfnür, P. Feulner, and D. Menzel. *A study of the adsorption sites of hydrogen on Ru(001) at saturation coverage by electron reflection*. Surf. Sci. **180**, (1987) 237.
- [Lin87b] M. Lindroos, H. Pfnür, and D. Menzel. *Investigation of a disordered adsorption system by electron reflection: H/Ru(001) at intermediate coverages*. Surf. Sci. **192**, (1987) 421.
- [Lis04] M. Lisowski, P. Loukakos, U. Bovensiepen, J. Stähler, C. Gahl, and M. Wolf. *Ultra-fast dynamics of electron thermalization, cooling and transport effects in Ru(001)*. Appl. Phys. A **78**, (2004) 165.
- [Lis05] M.J. Lisowski. *Elektronen- und Magnetisierungsdynamik in Metallen untersucht mit zeitaufgelöster Photoemission*. Ph.D. thesis, Freie Universität Berlin, Fachbereich Physik (2005).
- [Liv00] T. Livneh and M. Asscher. *The adsorption and Decomposition of C₂H₄ on Ru(001): A combined TPR and Work Function Change Study*. J. Phys. Chem. B **104**, (2000) 3355.

- [Lun05] A.C. Luntz and M. Persson. *How adiabatic is activated adsorption/associative desorption?* J. Chem. Phys. **123**, (2005) 074704.
- [Lun06] A.C. Luntz, M. Persson, S. Wagner, C. Frischkorn, and M. Wolf. *Femtosecond laser induced associative desorption of H₂ from Ru(0001): Comparison of “first principles” theory with experiment.* J. Chem. Phys. **124**, (2006) 244702.
- [Lup] M. Luppi, R.A. Olsen, and E.J. Baerends. *Ab-initio six-dimensional potential energy surface for H₂ on clean Ru(001).* Phys. Rev. B (to be published).
- [Mad75] T.E. Madey, H.A. Engelhardt, and D. Menzel. *Adsorption of oxygen and oxidation of CO on the ruthenium (001) surface.* Surf. Sci. **48**, (1975) 304.
- [Mad78] O. Madelung. *Solid State Theory.* Springer, Berlin (1978).
- [Mad86] T.E. Madey. *Electron- and Photon-Stimulated Desorption: Probes of Structure and Bonding at Surfaces.* Science **234**, (1986) 316.
- [Mah79] R. Mahon, T.J. McIlrath, V.P. Myerscough, and D.W. Koopman. *Third-Harmonic Generation in Argon, Krypton and Xenon: Bandwidth Limitations in the Vicinity of Lyman- α .* IEEE J. Quantum Electronics **15**, (1979) 444.
- [Mav98] M. Mavrikakis, B. Hammer, and J.K. Nørskov. *Effect of Strain on the Reactivity of Metal Surfaces.* Phys. Rev. Lett. **81**, (1998) 2819.
- [Mav99] M. Mavrikakis, L.B. Hansen, J.J. Mortensen, B. Hammer, and J.K. Nørskov. *Dissociation of N₂, NO and CO on Transition Metal Surfaces.* In D.G. Truhlar and K. Morokuma (Editors), *Transition State Modeling for Catalysis*, page 245. ACS Symp. Ser. 721 (1999).
- [Mei86] W. Meier, G. Ahlers, and H. Zacharias. *State selective population of H₂($v'' = 1, J'' = 1$) and D₂($v'' = 1, J'' = 2$) and rotational relaxation in collisions with H₂, D₂, and He.* J. Chem. Phys. **85**, (1986) 2599.
- [Men64] D. Menzel and R. Gomer. *Desorption from Metal Surfaces by Low-Energy Electrons.* J. Chem. Phys. **41**, (1964) 3311.
- [Men75] D. Menzel. *Desorption Phenomena.* In R. Gomer (Editor), *Topics in Applied Physics*, volume 4. Springer, Berlin (1975).
- [Mis92] J.A. Misewich, T.F. Heinz, and D.M. Newns. *Desorption induced by multiple electronic transitions.* Phys. Rev. L **68**, (1992) 3737.
- [Mis94] J.A. Misewich, A. Kalamarides, T.F. Heinz, U. Höfer, and M.M.T. Loy. *Vibrationally assisted electronic desorption: Femtosecond surface chemistry of O₂/Pd(111).* J. Chem. Phys. **100**, (1994) 736.
- [Mis95] J.A. Misewich, T.F. Heinz, P. Weigand, and A. Kalamarides. *Femtosecond surface science: the dynamics of desorption.* In H.-L. Dai, W. Ho (Editor), *Laser Spectroscopy and Photochemistry on Metal Surfaces*, page 764. World Scientific, Singapore (1995).

Bibliography

- [Mor92] M. Morin, N.J. Levinos, and A.L. Harris. *Vibrational energy transfer of CO/Cu(100): Nonadiabatic vibration/electron coupling*. J. Chem. Phys. **96**, (1992) 3950.
- [Mur99] M.J. Murphy, J.F. Skelly, A. Hodgson, and B. Hammer. *Inverted vibrational distributions from N₂ recombination at Ru(001): Evidence for a metastable molecular chemisorption well*. J. Chem. Phys. **110**, (1999) 6954.
- [Mus82] R.G. Musket, W. McLean, C.A. Colmenares, D.M. Makowiecki, and W.J. Siekhaus. *Preparation of atomically clean surfaces of selected elements: a review*. Appl. Surf. Sci. **10**(2), (1982) 143.
- [New91] D.M. Newns, T.F. Heinz, and J.A. Misewich. *Desorption by Femtosecond Laser Pulses: An Electron-Hole Effect?* Prog. Theor. Phys. Suppl. **106**, (1991) 411.
- [Nie02] H. Nienhaus. *Electronic excitation by chemical reactions on metal surfaces*. Surf. Sci. Rep. **45**, (2002) 1.
- [Noo87] I. NoorBatcha and R.R. Lucchese. *Effects of gas-phase collisions on particles rapidly desorbed from surfaces*. Phys. Rev. B **36**, (1987) 4978.
- [Ove98] H. Over. *Crystallographic study of interaction between adspecies on metal surfaces*. Prog. Surf. Sci. **58**, (1998) 249.
- [Par83] D.H. Parker. *Laser Ionization Spectroscopy and Mass Spectrometry*. In D.S. Kliger (Editor), *Ultrasensitive Laser Spectroscopy*, page 283. World Scientific, New York (1983).
- [Pfn83] H. Pfnür, P. Feulner, and D. Menzel. *The Influence of adsorbate Interactions on Kinetics and Equilibrium for CO on Ru(001). II. Desorption Kinetics and Equilibrium*. J. Chem. Phys. **79**, (1983) 4613.
- [Pis74] C. Pisani, G. Rabino, and F. Ricca. *Statistical analysis and model determination for thermal desorption spectra: Nitrogen on tungsten*. Surf. Sci. **41**, (1974) 277.
- [Pol72] J.C. Polanyi. *Some Concepts in Reaction Dynamics*. Acct. Chem. Res. **5**, (1972) 161.
- [Pry90] J.A. Prybyla, T.F. Heinz, J.A. Misewich, M.M.T. Loy, and J.H. Glowina. *Desorption induced by femtosecond laser pulses*. Phys. Rev. Lett. **64**, (1990) 1537.
- [Rab75] H. Rabitz and S.-H. Lam. *Rotational energy relaxation in molecular hydrogen*. J. Chem. Phys. **63**, (1975) 3532.
- [Red62] P.A. Redhead. *Thermal Desorption of Gases*. Vacuum **12**, (1962) 203.
- [Red64] P.A. Redhead. *Interaction of slow Electrons with Chemisorbed Oxygen*. Can. J. Phys. **42**, (1964) 886.
- [Rei65] F. Reif. *Grundlagen der Physikalischen Statistik und der Physik der Wärme*. de Gruyter (1965).

- [Rei95] G.A. Reider and T.F. Heinz. *Nonlinear Optical Effects at Surfaces and Interfaces: Recent Advances*. In P. Halewi (Editor), *Photonic Probes of Surfaces*, volume 2. Elsevier Science, Amsterdam (1995).
- [Ren89] K.D. Rendulic, G. Anger, and A. Winkler. *Wide range nozzle beam adsorption data for the systems $H_2/nickel$ and $H_2/Pd(100)$* . Surf. Sci. **208**, (1989) 404.
- [Ret02] B. Rethfeld, A. Kaiser, M. Vicanek, and G. Simon. *Ultrafast dynamics of nonequilibrium electrons in metals under femtosecond laser irradiation*. Phys. Rev. B. **65**, (2002) 214303.
- [Ris89] H. Risken. *The Fokker-Planck Equation*. Springer, Berlin (1989).
- [Rut02a] M. Rutkowski. *Untersuchung der mikroskopischen Dynamik der katalytischen D_2 -Reaktionen an $S/Pd(100)$ mit zustandsselektiver Laserspektroskopie*. Ph.D. thesis, Westfälische Wilhelms-Universität Münster, Fachbereich Physik (2002).
- [Rut02b] M. Rutkowski, D. Wetzig, H. Zacharias, and A. Groß. *Rotational and vibrational population of D_2 desorbing from sulfur-covered $Pd(100)$* . Phys. Rev. B **66**, (2002) 115405.
- [Sch81] H. Schober and P.H. Dederichs. *Phonon States of Elements. Electron States and Fermi surfaces of Alloys*. In *Landolt Börnstein New Series*, volume III/13a. Springer, Berlin (1981).
- [Sch92] L. Schröter, C. Trame, R. David, and H. Zacharias. *State specific velocity distribution of hydrogen isotopes desorbing from $Pd(100)$* . Surf. Sci. **272**, (1992) 229.
- [Sch00] M. Scheffler and C. Stampfl. *Theory of Adsorption on Metal Substrates*, volume II of *Handbook of Surface Science*, page 285. Elsevier, Amsterdam (2000).
- [Seh99] J. Sehested, C.J.H. Jacobsen, E. Törnquist, S. Rokni, and P. Stoltze. *Ammonia Synthesis over a Multipromoted Iron Catalyst: Extended Set of Activity Measurements, Microkinetic Model, and Hydrogen Inhibition*. J. Catal. **188**, (1999) 83.
- [She84] Y.R. Shen. *The Principles of Nonlinear Optics*. Wiley & Sons, New York (1984).
- [She89] Y.R. Shen. *Surface properties probed by second-harmonic and sum-frequency generation*. Nature **337**, (1989) 519.
- [Shi80a] S.-K. Shi and J.M. White. *Adsorption of O_2 and N_2O on carbon-covered $Ru(001)$ surfaces*. J. Chem. Phys. **73**, (1980) 5889.
- [Shi80b] H. Shimizu, K. Christmann, and G. Ertl. *Model studies on bimetallic Cu/Ru catalysts : II. Adsorption of hydrogen*. J. Catalysis **61**, (1980) 412.
- [Shi85] C. Shincho, E. Egawa, S. Naito, and K. Tamaru. *The behaviour of CO adsorbed on $Ru(1,1,10)$ and $Ru(001)$; the dissociation of CO at the step sites of the $Ru(1,1,10)$ surface*. Surf. Sci. **149**, (1985) 1.
- [Sok91] M. Sokolowski, T. Koch, and H. Pfnür. *Ordered structures and phase diagram of atomic hydrogen chemisorbed on ruthenium (001)*. Surf. Sci. **243**, (1991) 261.

Bibliography

- [Sta96] C. Stampfl, C. Schwegmann, H. Over, M. Scheffler, and G. Ertl. *Structure and Stability of a High-Coverage (11) Oxygen Phase on Ru(0001)*. Phys. Rev. Lett. **77**, (1996) 3371.
- [Sto51] H.H. Storch, N. Columbic, and R.B. Anderson. *The Fischer-Tropsch and Related Synthesis*. Wiley, New York (1951).
- [Str96] L.M. Struck, L.J. Richter, S.A. Buntin, R.R. Cavanagh, and J.C. Stephenson. *Femtosecond Laser-Induced Desorption of CO from Cu(100): Comparison of Theory and Experiment*. Phys. Rev. Lett. **77**, (1996) 4576.
- [Sun89] Y.-K. Sun and W.H. Weinberg. *Determination of the absolute saturation coverage of hydrogen on Ru(001)*. Surf. Sci. **214**, (1989) L246.
- [Tra03] J.R. Trail, D.M. Bird, M. Persson, and S. Holloway. *Electron-hole pair creation by atoms incident on a metal surface*. J. Chem. Phys. **119**, (2003) 4539.
- [Tul76] J.C. Tully. *Nonadiabatic Processes in Molecular Collisions*. In W.H. Miller (Editor), *Dynamics of Molecular Collisions*, volume B. Plenum Press, New York (1976).
- [Tul80] J.C. Tully. *Dynamics of gas-surface interactions: 3D generalized Langevin model applied to fcc and bcc surfaces*. J. Chem. Phys. **73**, (1980) 1975.
- [Tul81] J.C. Tully. *Dynamics of gas-surface interactions: Thermal desorption of Ar and Xe from platinum*. Surf. Sci. **111**, (1981) 461.
- [Tul00] J.C. Tully. *Chemical Dynamics at Metal Surfaces*. Annu. Rev. Phys. Chem. **51**, (2000) 153.
- [Vin05] J.K. Vincent, R.A. Olsen, G.-J. Kroes, M. Luppi, and E.-J. Baerends. *Six-dimensional quantum dynamics of dissociative chemisorption of H₂ on Ru(001)*. J. Chem. Phys. **122**, (2005) 044701.
- [Wag05] S. Wagner, C. Frischkorn, M. Wolf, M. Rutkowski, H. Zacharias, and A.C. Luntz. *Energy partitioning in the femtosecond-laser-induced associative D₂ desorption from Ru(001)*. Phys. Rev. B **72**, (2005) 205404.
- [Wea81] J.H. Weaver, C. Krafka, D.W. Lynch, and E.E. Koch. *Physics Data - Optical Properties of Metals*. Fachinformationszentrum Karlsruhe (1981).
- [Wet01] D. Wetzig, M. Rutkowski, H. Zacharias, and A. Groß. *Vibrational and rotational population distribution of D₂ associatively desorbing from Pd(100)*. Phys. Rev. B **63**, (2001) 205412.
- [Whi05] J.D. White, J. Chen, D. Matsiev, D.J. Auerbach, and A.M. Wodtke. *Conversion of large-amplitude vibration to electron excitation at a metal surface*. Nature **433**, (2005) 503.
- [Wil80] R.F. Willis. *Vibrational Spectroscopy of Adsorbates*. In *Springer Series in Chemical Physics*, volume 15. Springer, Berlin (1980).
- [Wil96] S. Wilke and M. Scheffler. *Potential-energy surface for H₂ dissociation over Pd(100)*. Phys. Rev. B **53**, (1996) 4926.

- [Wis83] H. Wise and J.G. McCarthy. *Thermodynamic properties of surface carbon on ruthenium*. Surf. Sci. **133**, (1983) 311.
- [Wol98] M. Wolf, M Aeschlimann. *Femtosekunden-Dynamik in Metallen - das kurze Leben heißer Elektronen*. Phys. Bl. **54**, (1998) 145.
- [Wur95] S. Wurm, P. Feulner, and D. Menzel. *Extremely High Vibrational Excitation of CO Molecules Desorbed from Transition Metal Surfaces by Electron Impact*. Phys. Rev. Lett. **74**, (1995) 2591.
- [Wur98] S. Wurm, P. Feulner, and D. Menzel. *Electron stimulated desorption of CO molecules from chemisorbed CO layers on Ru(001): a comparison of the distributions of translational and internal energies*. Surf. Sci. **400**, (1998) 155.
- [Xu05] L. Xu, H.Y. Xiao, and X.T. Zu. *Hydrogen adsorption on Ru(001) surface from density-functional periodic calculations*. Chem. Phys. **315**, (2005) 155.
- [Yat98] J.T. Yates. *Experimental Innovations in Surface Science*. Springer (1998).
- [Zam96] T. Zambelli, J. Wintterlin, J. Trost, and G. Ertl. *Identification of the "Active Sites" of a Surface-Catalyzed Reaction*. Science **273**, (1996) 1688.
- [Zap81] W. Zapka, D. Cotter, and Brackmann U. *Dye laser frequency tripling at 106 nm*. Opt. Comm. **36**, (1981) 79.
- [Zar88] R.N. Zare. *Angular Momentum*. Wiley and Sons (1988).
- [Zew94] A.H. Zewail. *Femtochemistry: Ultrafast dynamics of the chemical bond, Vol. I+II*. World Scientific, Singapore (1994).
- [Zim94] F.M. Zimmermann and W. Ho. *Velocity distributions of photochemically desorbed molecules*. J. Chem. Phys. **10**, (1994) 7700.
- [Zim95] F.M. Zimmermann and W. Ho. *State resolved studies of photochemical dynamics at surfaces*. Surf. Sci. Rep. **22**, (1995) 119.
- [Zub02] T. Zubkov, G.A. Morgan Jr., and J.T. Yates Jr. *Spectroscopic detection of CO dissociation on defect sites on Ru(109): implications for Fischer-Tropsch catalytic chemistry*. Chem. Phys. L. **362**, (2002) 181.
- [Zub03] T. Zubkov, G.A. Morgan Jr., J.T. Yates Jr., O. Köhlert, M. Lisowski, R. Schillinger, D. Fick, and H.J. Jänsch. *The effect of atomic steps on adsorption and desorption of CO on Ru(109)*. Surf. Sci. **526**, (2003) 57.

