

- [1] K. Al-Shamery, I. Beauport, B. Baumeister, T. Klüner, Th. Mull, M. Menges, C. Fischer, H.-J. Freund, P. Andresen, J. Freitag, V. Staemmler, Proceedings of the SPIE'S OE/LASER '94 conference, 2125, 182 (1994): State and spatially resolved studies of the UV-laser-induced desorption of molecules from oxide surfaces.
- [2] T. Klüner*, H.-J. Freund, J. Freitag, V. Staemmler, J. Chem. Phys. **104** (1996), 10030: Laser-induced desorption of NO from NiO(100): Ab initio calculations of potential surfaces for intermediate excited states.
- [3] U.J. Katter, T. Risse, H. Schlienz, M. Beckendorf, T. Klüner, H. Hamann, H.-J. Freund, J. Magn. Res. **126** (1997), 242: ESR and TPD Investigations of the Adsorption of Di-tert.-butyl-nitroxide (DTBN) on Au(111) and NiO(111): Evidence for Long Range Interactions.
- [4] U.J. Katter, T. Hill, T. Risse, H. Schlienz, M. Beckendorf, T. Klüner, H. Hamann, H.-J. Freund, J. Phys. Chem. B **101** (1997), 3776: Dynamics of the Stable Radical Di-tert.-butyl-nitroxide DTBN) on an Epitaxially Grown Al₂O₃ Film.
- [5] U.J. Katter, T. Hill, T. Risse, H. Schlienz, M. Beckendorf, T. Klüner, H. Hamann, H.-J. Freund, J. Phys. Chem. B **101** (1997), 552: Adsorption of the Stable Radical Di-tert.-butyl-nitroxide (DTBN) on an Epitaxially grown Al₂O₃ Film.
- [6] T. Klüner*, H.-J. Freund, J. Freitag, V. Staemmler, J. Mol. Catal. A **119** (1997), 155: Laser induced desorption of NO from NiO(100): Characterization of potential energy surfaces of excited states.
- [7] S. Thiel, T. Klüner*, M. Wilde, K. Al-Shamery, H.-J. Freund, Chem. Phys. **228** (1998), 185: The role of the initial population of molecular vibrations in surface photochemistry.
- [8] T. Klüner*, H.-J. Freund, V. Staemmler, R. Kosloff, Phys. Rev. Lett. **80** (1998), 5208: Theoretical investigation of laser induced desorption of small molecules from oxide surfaces: a first principles study.
- [9] T. Klüner*, S. Thiel, H.-J. Freund, V. Staemmler, Proceedings of the SPIE'S OE/LASER '98 conference, 3272, 177 (1998): Laser-Induced Desorption of NO from NiO(100): *Ab initio* and Wave Packet Calculations.
- [10] S. Thiel, T. Klüner*, H.-J. Freund, Chem. Phys. **236** (1998), 263: Interference-Effects in the Laser Induced Desorption of Small Molecules from Surfaces - a Model Study.
- [11] S. Thiel, T. Klüner*, H.-J. Freund, R. Kosloff, Isr. J. Chem. **38** (1998), 321: Velocity Distributions after Laser Induced Desorption of NO from NiO(100) -The role of the Angular Coordinate.
- [12] T. Klüner*, S. Thiel, V. Staemmler, H.-J. Freund, Chem. Phys. Lett. **294** (1998), 413: The vibrational excitation of NO desorbing from NiO(100) after UV laser irradiation: Is NO⁻ a possible intermediate species ?
- [13] T. Klüner*, S. Thiel, V. Staemmler, J. Phys. B: At. Mol. Opt. Phys. **32** (1999), 4931: Ab initio calculation of proton scattering from He(1s2s,¹S): a first-principles wavepacket study beyond the Born-Oppenheimer approximation.
- [14] H.-J. Freund, T. Klüner, R. Wichtendahl, S. Thiel, M. Adelt, W. Drachsel, M. Bäumer, H. Kuhlenbeck, T. Risse, K. Al-Shamery, M. Kampling, H. Hamann, NATO ASI Ser. Vol E, 2000, 91: Metal-Ligand Interactions in Chemistry, Physics and Biology: Molecules on Clean and Modified Oxide Surfaces.
- [15] T. Klüner, N. Govind, Y.A. Wang, E.A. Carter, Phys. Rev. Lett. **86** (2001), 5954: Prediction of Electronic Excited States of Adsorbates on Metal Surfaces from First Principles.
- [16] S. Thiel, M. Pykavy, T. Klüner*, H.-J. Freund, R. Kosloff, V. Staemmler, Phys. Rev. Lett. **87** (2001), 077601: Three-Dimensional *Ab initio* Quantum Dynamics of the Photodesorption of CO from Cr₂O₃(0001): Stereodynamic Effects.
- [17] T. Klüner, N. Govind, Y.A. Wang E.A. Carter, J. Chem. Phys. **116** (2002), 42: Periodic density functional embedding theory for complete active space self-consistent field and configuration interaction calculations: Ground and excited states.
- [18] S. Thiel, M. Pykavy, T. Klüner*, H.-J. Freund, R. Kosloff, V. Staemmler, J. Chem. Phys. **116** (2002), 762: Rotational Alignment in the Photodesorption of CO from Cr₂O₃: A systematic three-dimensional *ab initio* study.

- [19] S. Borowski, S. Thiel, T. Klüner*, H.-J. Freund, R. Tisma, H. Lederer, Comp. Phys. Comm. **143** (2002), 162: High-dimensional quantum dynamics of molecules on surfaces: a massively parallel implementation.
- [20] C.P. Koch, T. Klüner, R. Kosloff, J. Chem. Phys. **116** (2002), 7983: A complete quantum description of an ultrafast pump-probe charge transfer event in condensed phase.
- [21] T. Klüner, N. Govind, Y.A. Wang, E. A. Carter, Phys. Rev. Lett. **88** (2002), 209702: Reply to the Comment on „Prediction of Electronic Excited States of Adsorbates on Metal Surfaces from First Principles“, Phys. Rev. Lett. **86**, 5954 (2001).
- [22] M. Pykavy, S. Thiel, T. Klüner*, J. Phys. Chem. B **106** (2002), 12556: Laser induced desorption of CO from Cr₂O₃(0001): ab initio calculation of the four dimensional potential energy surface for an intermediate excited state.
- [23] S. Thiel, T. Klüner*, D. Lemoine, H.-J. Freund, Chem. Phys. **282** (2002), 361: Rotational Preexcitation in the Photodesorption of CO from Cr₂O₃.
- [24] A. Delin, T. Klüner, Phys. Rev. B **66** (2002), 035117: Excitation spectra and ground-state properties from density functional theory for the inverted band-structure systems β-HgS, HgSe and HgTe.
- [25] C.P. Koch, T. Klüner*, H.-J. Freund, R. Kosloff, Phys. Rev. Lett. **90** (2003), 117601: Femtosecond photodesorption of NO from NiO(100): A theoretical investigation from first principles.
- [26] C.P. Koch, T. Klüner*, H.-J. Freund, R. Kosloff, J. Chem. Phys. **119** (2003), 1750: Surrogate Hamiltonian study of electronic relaxation in the femtosecond laser induced desorption of NO/NiO(100).
- [27] S.K. Shaikhutdinov, R. Meyer, D. Lahav, M. Bäumer, T. Klüner, H.-J. Freund, Phys. Rev. Lett., **91** (2003), 076102: Determination of Atomic Structure of the Metal-Oxide interface: Pd nanodeposits on an FeO(111) film.
- [28] C. Bach, T. Klüner, A. Groß, Chem. Phys. Lett. **376** (2003), 424: Simulation of laser induced desorption of NO from NiO(100).
- [29] C.P. Koch, T. Klüner*, H.-J. Freund, R. Kosloff, Virtual Journal of Ultrafast Science Volume 2, Issue 4: Femtosecond photodesorption of NO from NiO(100): A theoretical investigation from first principles.
- [30] T. Risse, A. Carlsson, M. Bäumer, T. Klüner, H.-J. Freund, Surf. Sci. Lett. **546** (2003), L829: Using IR intensities as a probe for studying the surface chemical bond.
- [31] C.P. Koch, T. Klüner*, H.-J. Freund, R. Kosloff, Virtual Journal of Ultrafast Science Volume 2, Issue 8: Surrogate Hamiltonian study of electronic relaxation in the femtosecond laser induced desorption of NO/NiO(100).
- [32] S. Borowski, T. Klüner*, H.-J. Freund, J. Chem. Phys. **119** (2003), 10367: Complete analysis of the angular momentum distribution for molecules desorbing from a surface.
- [33] S. Borowski, T. Klüner*, H.-J. Freund, I. Klinkmann, K. Al-Shamery, M. Pykavy, V. Staemmler, Appl. Phys. A **78** (2004), 223: Lateral velocity distributions in laser induced desorption of CO from Cr₂O₃(0001): Experiment and Theory.
- [34] C. Bach, T. Klüner, A. Groß, Appl. Phys. A **78** (2004), 231: Multidimensional mixed quantum-classical description of the laser-induced desorption of molecules.
- [35] G. Pacchioni, C. Di Valentin, D. Dominguez-Ariza, F. Illas, T. Bredow, T. Klüner, V. Staemmler, J. Phys: Condens. Matter **16** (2004), S2497: Bonding of NH₃, CO and NO to NiO and Ni-doped MgO: a problem for density functional theory.
- [36] T. Klüner*, Nachr. Chem. **52** (2004), 313: Trendbericht Theoretische Chemie 2003: Theoretische Untersuchungen an Oberflächen.
- [37] S. Borowski, T. Klüner*, Chem. Phys. **304** (2004), 51: Massively parallel Hamiltonian action in pseudospectral algorithms applied to quantum dynamics of laser induced desorption.

- [38] T. Klüner*, Isr. J. Chem., **45** (2005), 77: Laser induced desorption of small molecules from oxide surfaces: A first principles study.
- [39] A. Cörper, G. Bozdech, N. Ernst, T. Klüner, H.-J. Freund, Phys. Stat. Sol. (b) **242** (2005), 2462: Field electron energy spectroscopy of alumina supported platinum adatoms.
- [40] R. Meyer, D. Lahav, T. Schalow, M. Laurin, B. Brandt, S. Schauermann, S. Guimond, T. Klüner, H. Kuhlenbeck, J. Libuda, Sh. Shaikhutdinov, H.-J. Freund, Surf. Sci. **586** (2005), 174: CO adsorption and thermal stability of Pd deposited on a thin FeO(111) film.
- [41] M. Morkel, H. Unterhalt, T. Klüner, G. Rupprechter, H.-J. Freund, Surf. Sci. **586** (2005), 146: Interpreting intensities in vibrational sum frequency generation (SFG) spectroscopy: CO adsorption on Pd surfaces
- [42] D. Kröner, I. Mehdaoui, H.-J. Freund, T. Klüner*, Chem. Phys. Lett. **415** (2005), 150: Three-dimensional ab initio simulation of laser-induced desorption of NO from NiO(100)
- [43] D.E. Starr, F. M.T. Mendes, J. Middeke, R.-P. Blum, H. Niehus , D. Lahav, S. Guimond, A. Uhl, T. Klüner, M. Schmal, H. Kuhlenbeck, S. Shaikhutdinov, H.-J. Freund, Surf. Sci. **599** (2005), 14: Preparation and characterization of well-ordered, thin niobia films on a metal substrate.
- [44] S. Dittrich, H.-J. Freund, C.P. Koch, R. Kosloff , T. Klüner*, J. Chem. Phys., in press: Two-dimensional surrogate Hamiltonian investigation of laser induced desorption of NO/NiO(100).
- [45] I. Mehdaoui, D. Kröner, M. Pykavy, H.-J. Freund, T. Klüner*, Phys. Chem. Chem. Phys., in press: Photo-induced desorption of NO from NiO(100): Calculation of the four-dimensional potential energy surfaces and systematic wave packet studies.