

## Publications Dr. Markus Drees

### Scientific Articles

- 59) W. R. Heinz, T. Kratky, M. Drees, A. Wimmer, O. Tomanec, S. Guenther, M. Schuster, R. A. Fischer, 'Mixed precious-group metal-organic frameworks: a case study of the HKUST-1 analogue [RuxRh<sub>3-x</sub>(BTC)<sub>2</sub>]', *Dalton Trans.*, **48(32)**, 12031-12039 (2019). DOI: [10.1039/c9dt01198f](https://doi.org/10.1039/c9dt01198f)
- 58) J. Mink, A. Stirling, D.O. Ojwang, G Svensson, J. Mihaly, C. Nemeth, M. Drees, L. Hajba, 'Vibrational properties and bonding analysis of copper hexacyanoferrate complexes in solid state', *Appl. Spectroscopy Rev.*, **54(5)**, 369-424 (2019). DOI: [10.1080/05704928.2018.1459659](https://doi.org/10.1080/05704928.2018.1459659)
- 57) B. J. Hofmann, S. Huber, R. M. Reich, M. Drees, F. E. Kühn, 'Ethyltrioxorhenium - Catalytic application and decomposition pathways', *J. Organomet. Chem.*, **885(1)**, 32-38 (2019). DOI: [10.1016/j.jorganchem.2019.02.004](https://doi.org/10.1016/j.jorganchem.2019.02.004)
- 56) S. Frischhut, F. Kaiser, W. Klein, M. Drees, F. E. Kühn, T.F. Fässler, 'Capping nido-Nonagermanide Clusters with M-PPh<sub>3</sub> and Dynamics in Solution: Synthesis and Structure of closo-[(Me<sub>3</sub>Si)<sub>3</sub>Si]<sub>3</sub>Et[Ge<sub>9</sub>M](PPh<sub>3</sub>) (M = Ni, Pt)', *Organometallics*, **37(24)**, 4560-4567 (2018). DOI: [10.1021/acs.organomet.8b00459](https://doi.org/10.1021/acs.organomet.8b00459)
- 55) M. Weger, M.M. Giuman, M.G. Knaus, M. Ackermann, M. Drees, J. Hornung, P.J. Altmann, R.A. Fischer, B. Rieger, 'Single-Site, Organometallic Aluminum Catalysts for the Precise Group Transfer Polymerization of Michael-Type Monomers', *Chem Eur. J.*, **24(56)**, 14950-14957 (2018). DOI: [10.1002/chem.201802075](https://doi.org/10.1002/chem.201802075)
- 54) M.R. Machat, A. Fischer, D. Schmitz, M. Vöst, M. Drees, C. Jandl, A. Pöthig, N.P.M. Casati, W. Scherer, B. Rieger, 'Behind the Scenes of Group 4 Metallocene Catalysis: Examination of the Metal-Carbon Bond', *Organometallics*, **37(16)**, 2690-2705 (2018). DOI: [10.1021/acs.organomet.8b00339](https://doi.org/10.1021/acs.organomet.8b00339)
- 53) J. Mink, S.L.M.Goh, M.P.Högerl, F.E.Kühn, M. Drees, J. Mihály, C. Németh, L. Hajba, 'Structure and vibrational spectroscopic study of phthalimido-functionalized N-heterocyclic palladium complexes. Correlations between structure and catalytic activity', *J. Organomet. Chem.*, **896(1)**, 233-250 (2018). DOI: [10.1016/j.jorganchem.2018.01.047](https://doi.org/10.1016/j.jorganchem.2018.01.047)
- 52) S. Frischhut, W. Klein, M. Drees, T.F. Fässler, 'Acylation of Homoatomic Ge<sub>9</sub> Cages and Subsequent Decarbonylation', *Chem Eur. J.*, **24(36)**, 9009-9014 (2018). DOI: [10.1002/chem.201802318](https://doi.org/10.1002/chem.201802318)
- 51) A. M. Arnold, A. Poethig, M. Drees, T. Gulder, 'NXS, Morpholine, and HFIP: The Ideal Combination for Biomimetic Haliranium-Induced Polyene Cyclizations', *J. Am. Chem. Soc.*, **140(12)**, 4344-4353 (2018). DOI: [10.1021/jacs.8b00113](https://doi.org/10.1021/jacs.8b00113)
- 50) M. R. Machat, D. Lanzinger, M. Drees, Markus, P. J. Altmann, E. Herdtweck, B. Rieger, 'High-Melting, Elastic Polypropylene: A One-Pot, One-Catalyst Strategy toward Propylene-Based Thermoplastic Elastomers', *Macromolecules*, **51(3)**, 914-929 (2018). DOI: [10.1021/acs.macromol.7b02679](https://doi.org/10.1021/acs.macromol.7b02679)
- 49) S. M. Balasekaran, A. Hagenbach, M. Drees, U. Abram, '[TcII(NO)(trifluoroacetate)<sub>4</sub>F]<sup>2-</sup> - synthesis and reactions', *Dalton Trans.*, **46(39)**, 13544-13552 (2017). DOI: [10.1039/c7dt03084c](https://doi.org/10.1039/c7dt03084c)

- 48) A.C. Lindhorst, M. Drees, W. Bonrath, J. Schuetz, T. Netscher, F.E. Kühn, Mechanistic insights into the biomimetic catalytic hydroxylation of arenes by a molecular Fe(NHC) complex', *J. Catal.*, **352**, 599-605 (2017). DOI: [10.1016/j.jcat.2017.06.018](https://doi.org/10.1016/j.jcat.2017.06.018)
- 47) D. S. Morris, C. Weetman, J.T.C. Wennmacher, M. Cokoja, M. Drees, F.E. Kühn, J.B. Love, 'Reduction of carbon dioxide and organic carbonyls by hydrosilanes catalysed by the perrhenate anion', *Catal. Sci. Technol.*, **7(13)**, 2838-2845 (2017). DOI: [10.1039/C7CY00772H](https://doi.org/10.1039/C7CY00772H)
- 46) J. Richers, M. Heilmann, M. Drees, K. Tiefenbacher, 'Synthesis of Lactones via C-H Functionalization of Nonactivated C(sp<sup>3</sup>)-H Bonds', *Org. Lett.*, **18(24)**, 6472-2875 (2016). DOI: [10.1021/acs.orglett.6b03371](https://doi.org/10.1021/acs.orglett.6b03371)
- 45) D. Jantke, L. Pardatscher, M. Drees, M. Cokoja, W. A. Herrmann, F. E. Kühn, 'Hydrogen Production and Storage on a Formic Acid/Bicarbonate Platform using Water-Soluble N-Heterocyclic Carbene Complexes of Late Transition Metals', *ChemSusChem*, **9(19)**, 2849-2854 (2016). DOI: [10.1002/cssc.201600861](https://doi.org/10.1002/cssc.201600861)
- 44) A. Schmidt, M. Hollering, M. Drees, A. Casini, F.E. Kühn, 'Supramolecular exo-functionalized palladium cages: fluorescent properties and biological activity', *Dalton Trans.*, **45(20)**, 8556-8565. DOI:[10.1039/c6dt00654j](https://doi.org/10.1039/c6dt00654j)
- 43) N. Grover, M. Drees, F. E. Kühn, 'Oxidation of [CpMo(CO)<sub>3</sub>R] olefin epoxidation precatalysts with tert-butylhydroperoxide', *J. Catal.*, **329**, 269-285 (2015). DOI: [10.1016/j.jcat.2015.05.019](https://doi.org/10.1016/j.jcat.2015.05.019)
- 42) M. H. Anthofer, M. E. Wilhelm, M. Cokoja, M. Drees, W. A. Herrmann, F. E. Kühn, 'Hydroxy-Functionalized Imidazolium Bromides as Catalysts for the Cycloaddition of CO<sub>2</sub> and Epoxides to Cyclic Carbonates', *ChemCatChem*, **7(1)**, 94-98 (2015). DOI: [10.1002/cctc.201402754](https://doi.org/10.1002/cctc.201402754)
- 41) N. Eckstein, L.A. Jantke, T.F. Fässler, J. Mink, M. Drees, T. Nilges, 'Structure and Vibrational Analyses of LiP<sub>15</sub>', *Eur. J. Inorg. Chem.*, **(30)**, 5135-5144 (2014). DOI: [10.1002/ejic.201402383](https://doi.org/10.1002/ejic.201402383)
- 40) V. D'Elia, A. Abdul-Ghani, A. Monassier, J. Sofack-Kreuzer, J. D. A. Pelletier, M. Drees, S. V. C. Vummaleti, A. Poater, L. Cavallo, M. Cokoja, J.M. Basset, F. E. Kühn, 'Dynamics of the NbCl<sub>5</sub>-Catalyzed Cycloaddition of Propylene Oxide and CO<sub>2</sub>: Assessing the Dual Role of Nucleophilic Co-catalysts', *Chem. Eur. J.*, **20(37)**, 11870-11882 (2014). DOI: [10.1002/chem.201400324](https://doi.org/10.1002/chem.201400324)
- 39) S. M. Balasekaran, J. Spandl, A. Hagenbach, K. Köhler, M. Drees, U. Abram, 'Fluoridonitrosyl Complexes of Technetium(I) and Technetium(II). Synthesis, Characterization, Reactions, and DFT Calculations', *Inorg. Chem.*, **53(10)**, 5117-5128 (2014). DOI:[10.1021/ic500229r](https://doi.org/10.1021/ic500229r)
- 38) R. G. Harms, I. I. E. Markovits, M. Drees, W. A. Herrmann, M. Cokoja, F. E. Kühn, 'Cleavage of C-O Bonds in Lignin Model Compounds Catalyzed by Methylidioxorhenium in Homogeneous Phase', *ChemSusChem*, **7(2)**, 429-434 (2014). DOI:[10.1002/cssc.201300918](https://doi.org/10.1002/cssc.201300918)
- 37) S. J. Hock, L.-A. Schaper, A. Poethig, M. Drees, E. Herdtweck, O. Hiltner, W. A. Herrmann, F. E. Kühn, 'Synthesis and characterisation of chelated cationic ReI(CO)<sub>3</sub>bis(NHC)(WCA) complexes', *Dalton Trans.*, **43(5)**, 2259-2271 (2014). DOI:[10.1039/c3dt52605d](https://doi.org/10.1039/c3dt52605d)

- 36) J. Ziriakus, T. K. Zimmermann, A. Poethig, M. Drees, S. Haslinger, D. Jantke, F. E. Kühn, 'Ruthenium-Catalyzed Transvinylolation - New Insights', *Adv. Synth. Cat.*, **355(14-15)**, 2845-2859 (2013).  
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- 35) D. Jantke, M. Cokoja, M. Drees, W. A. Herrmann, F. E. Kühn, 'Ruthenium-Catalyzed Hydrogenation of Oxygen-Functionalized Aromatic Compounds in Water', *ChemCatChem*, in print.  
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- 34) A. N. Marziale, A. Friedrich, I. Klopsch, M. Drees, V. R. Celinski, J. Schmedt auf der Guenne, S. Schneider, 'The Mechanism of Borane-Amine Dehydrocoupling with Bifunctional Ruthenium Catalysts', *J. Am. Chem. Soc.*, **135(36)**, 13342-13355 (2013).  
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- 33) S.A. Reindl, A. Poethig, M. Drees, B. Bechlars; E. Herdtweck,; W.A. Herrmann, F. E. Kühn, 'Pyrazolato-Bridged Dinuclear Complexes of Ruthenium(II) and Rhodium(III) with N-Heterocyclic Carbene Ligands: Synthesis, Characterization, and Electrochemical Properties' *Organometallics*, **32(15)**, 4082-4091 (2013).  
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- 32) M. Drees, S.A. Hauser, M. Cokoja, F.E. Kühn, 'DFT studies on the reaction pathway of the catalytic olefin epoxidation with CpMoCF<sub>3</sub> dioxo and oxo-peroxo complexes', *J. Organomet. Chem.*, **748**, 36-45 (2013).  
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- 31) L.A. Schaper, W. Xuhui, P.J. Altmann, K. Oefele, A. Poethig, M. Drees, J. Mink, E. Herdtweck, B. Bechlars, W.A. Herrmann, F.E. Kühn, 'Synthesis and Comparison of Transition Metal Complexes of Abnormal and Normal Tetrazolylenes: A Neglected Ligand Species', *Inorg. Chem.*, **52(12)**, 7031-7044 (2013).  
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- 30) S. Huber, M. Cokoja, M. Drees, J. Mink, F. E. Kühn, 'Xylyltrioxorhenium – the first arylrhenium(VII) oxide applicable as an olefin epoxidation catalyst', *Cat. Scien Tech.* **3(2)**, 388-393 (2013).  
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- 29) S. A. Hauser, M. Cokoja, M. Drees, F. E. Kühn, 'Catalytic olefin epoxidation with a fluorinated organomolybdenum complex', *J. Mol. Cat. A*, **363-364**, 237-244 (2012).  
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- 28) P. Gigler, M. Drees, K. Riener, B. Bechlars, W. A. Herrmann, F. E. Kühn, 'Mechanistic insights into the hydrosilylation of allyl compounds – Evidence for different coexisting reaction pathways', *J. Catal.*, **295**, 1-14 (2012).  
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- 27) M. Drees, M. Cokoja, F. E. Kühn, 'Recycling CO<sub>2</sub>? Computational Considerations of the Activation of CO<sub>2</sub> with Homogeneous Transition Metal Catalysts', *ChemCatChem*, **4**, 1703-1712 (2012).  
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- 26) L. A. Schaper, K. Oefele, R. Kadyrov, B. Bechlars, M. Drees, M. Cokoja, W. A. Herrmann, F. E. Kühn, 'N-Heterocyclic carbenes via abstraction of ammonia: 'normal' carbenes with 'abnormal' character', *Chem. Comm.*, **48 (32)**, 3857-3859 (2012).  
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- 24) M. Carril, P. Altmann, M. Drees, W. Bonrath, T. Netscher, J. Schütz, F. E. Kühn, 'Methyltrioxorhenium-catalyzed oxidation of pseudocumene for vitamin E synthesis: A study of solvent and ligand effects', *J. Catal.*, **283 (1)**, 55-67 (2011).  
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- 23) S. Y. T. Lee, M. Cokoja, M. Drees, Y. Li, J. Mink, W. A. Herrmann, F. E. Kühn, 'Transformation of Nickelalactones to Methyl Acrylate: On the Way to a Catalytic Conversion of Carbon Dioxide', *ChemSusChem.*, **4 (9)**, 1275-1279 (2011).  
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- 22) M. Drees, T. Strassner, 'The Etard Reaction: A DFT Study', *Inorg. Chem.*, **50 (12)**, 5833-5840 (2011).  
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- 21) O. Hiltner, F.J. Boch, L. Brewitz, P. Härter, M. Drees, E. Herdtweck, W. A. Herrmann, F. E. Kühn, 'Bridged fac-Tricarbonylrhodium(I)-Biscarbene Complexes: Synthesis, Characterization, and Molecular Dynamics', *Eur. J. Inorg. Chem.*, **(33)**, 5284-5293 (2010).  
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- 20) M. A. Fredericks, M. Drees, K. Köhler, 'Acceleration of the Rate of the Heck Reaction through UV- and Visible-Light-Induced Palladium(II) Reduction', *ChemCatChem*, **2 (11)**, 1467-1476 (2010).  
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- 19) A. Günyar, D. Betz, M. Drees, E. Herdtweck, F. E. Kühn, 'Highly soluble dichloro, dibromo and dimethyl dioxomolybdenum(VI)-bipyridine complexes as catalysts for the epoxidation of olefins', *J. Mol. Cat. A*, **331 (1-2)**, 117-124 (2010).  
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- 18) P. Maier, M. Toennis, G. Klinker, A. Raith, M. Drees, F. E. Kühn, 'What Do You Do When Two Hands Are Not Enough? Interactive Selection of Bonds Between Pairs of Tangible Molecules', *Proceedings of the 2010 IEEE Symposium on 3D User Interfaces*, 83-90 (2010).  
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- 17) A. Friedrich, M. Drees, J. Schmedt auf der Günne, S. Schneider, 'Hydrogen generation from small molecules using bifunctional Ruthenium complexes', *Preprints of Symposia - ACS Div. Fuel Chem.*, **55 (1)**, 278-279 (2010).
- 16) A. Friedrich, M. Drees, M. Kaess, E. Herdtweck, S. Schneider, 'Ruthenium Complexes with Cooperative PNP-Pincer Amine, Amido, Imine and Enamido Ligands: Facile Ligand Backbone Functionalization Processes', *Inorg. Chem.*, **49 (12)**, 5482-5494 (2010).  
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- 14) A. Friedrich, M. Drees, S. Schneider, 'Ruthenium-Catalyzed Dimethylamineborane Dehydrogenation: Stepwise Metal-Centered Dehydrocyclization', *Chem. Eur. J.*, **15(40)**,

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12) Z. Xu, M. Zhou, M. Drees, H. Chaffey-Millar, E. Herdtweck, W. A. Herrmann, F. E. Kühn, 'Mono- and Bis- Methyltrioxorhenium(VII) Complexes with Salen Ligands: Synthesis, Properties, Applications', *Inorg. Chem.*, **48 (14)**, 6812-6822 (2009).

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11) O. Hiltner, E. Herdtweck, M. Drees, W. A. Herrmann, F. E. Kühn, 'Synthesis and Characterization of Two New fac-Tricarbonylrhenium(I) Biscarbene Complexes', *Eur. J. Inorg. Chem.*, **(13)**, 1825-1831 (2009).

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10) W. Kleist, S. S. Pröckl, M. Drees, K. Köhler, L. Djarkovitch\*, 'Amination of Aryl Chlorides and Fluorides toward the Synthesis of Aromatic Amines by Palladium Catalyzed Route or Transition Metal Free Way: Scopes and Limitations', *J. Mol. Cat. A.*, **303 (1-2)**, 15-22 (2009).

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9) M. Käß, A. Friedrich, M. Drees, S. Schneider\*, 'Ruthenium Complexes with Cooperative PNP Ligands: Bifunctional Catalysts for the Dehydrogenation of Ammonia-Borane', *Angew. Chem Int. Ed., Angew. Chem. Int. Ed.*, **48 (5)**, 905-907 / *Angew. Chem.*, **121 (5)**, 922-924 (2009).

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8) M. Drees, T. Strassner\*, 'Mechanism of the MoO<sub>2</sub>Cl<sub>2</sub> Catalyzed Hydrosilylation - a DFT study', *Inorg. Chem.*, **46(25)**, 10850-10859 (2007).

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7) T. Segmüller, P. A. Schlüter, M. Drees, A. Schier, S. Nogai, N. W. Mitzel, T. Strassner\*, H.H. Karsch\*, 'Dianionic amidates at silicon and germanium Centers: Four-, six- and eight-membered rings', *J. Organomet. Chem.*, **692(13)**, 2789-2799 (2007).

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6) A. Netz, M. Drees, T. Strassner\*, T. J. J. Müller\*, 'Planar-Chiral Chromiumcarbonyl Arene Complex Substituted Propargyl Cationns - A Spectroscopic and Computational Study', *Eur. J. Org. Chem.*, 540-547 (2007).

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5) M. Drees, T. Strassner\*, 'Ruthenium Tetroxide Oxidations of Alkanes: DFT Calculations of Barrier Heights and Kinetic Isotope Effects', *J. Org. Chem.*, **71(5)**, 1755-1760 (2006). [+ Cover Design]

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4) D. Freitag, M. Drees, S. Goutal, T. Strassner\*, P. Metz\*, 'Synthetic and Computational Studies on Intramolecular [2+2] Sulfonyl Isocyanate-Olefin Cycloadditions', *Tetrahedron* **61(23)**, 5615-5621 (2005).

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3) T. Strassner\*, M. Drees, 'Rutheniumtetroxide Oxidation of Alkenes A Density Functional Theory Study', *Journal of Molecular Structure - THEOCHEM*, **671(1-3)**, 197-

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2) L. D. McPherson, M. Drees, S. I. Khan, T. Strassner\*, M.M. Abu-Omar\*, 'Multielectron Atom Transfer Reactions of Perchlorate and Other Substrates Catalyzed by Rhenium Oxazoline and Thiazoline Complexes: Reaction Kinetics, Mechanisms, and Density Functional Theory Calculations.', *Inorg. Chem.*, **43**, 4036-4050 (2004).

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1) M. Drees, L. Kleiber, M. Weimer, T. Strassner\*, 'A Computational Study of the Stereoselective Decarboxylation in the Synthesis of Naproxen', *Eur. J. Org. Chem.*, 2405-2410 (2002).

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### Lectures

- 1) "Stereoselective Synthesis of Naproxen - which Factors determine the Stereochemistry?" , 07.04.2002, ORGN-015, ACS Meeting, Orlando, FL (USA)
- 2) "What is the Active Chromium Species in the Alk(a/e)ne Oxidation?", 10.04.2002, INOR-371, ACS Meeting, Orlando, FL (USA)
- 3) "Calculations on Chromyl Chloride Oxidations and Naproxen", 28.09.2002, Houk group meeting, UCLA (USA)
- 4) "Project overview: ReO(hoz)<sub>2</sub> as oxygen transfer catalyst", 05.10.2002, Abu-Omar group meeting, UCLA (USA)
- 5) "DFT calculations as predictive tools for syntheses and mechanisms in (metal)organic chemistry ", 04.12.2006, Assessment Event, AstraZeneca, Macclesfield (UK)
- 6) "What experimentalists should know about computational chemistry Part I", 12.09.08, NanoCat Seminar, Technische Universitaet Munich, Garching (D)
- 7) "What experimentalists should know about computational chemistry Part II", 31.10.08, NanoCat Seminar, Technische Universitaet Munich, Garching (D)
- 8) "Metall-oxo compounds in catalysis: Activation of unreactive bonds", 08.01.09, CRC-Workshop "Computation in Catalysis", Technische Universitaet Munich, Garching (D)

### Posters

- 1) "Chromyl chloride, a DFT study of the Étard reaction", September 2003, Poster INOR-456, ACS Meeting, New York City, NY (USA)
- 2) "A density functional study about the oxidation of ethene with ruthenium tetroxide", March 2004, Poster INOR-585, ACS Meeting, Anaheim, CA (USA)

3) "Multielectron Atom Transfer Reactions of Pyridine-N-oxide and other substrates catalysed by Re-oxazoline: Mechanism and DFT-study", January 2005, WATOC Conference, Cape Town (Rep. South Africa)

4) "A Density Functional Study about the Oxidation of Ethene with Ruthenium Tetraoxide", January 2005, WATOC Conference, Cape Town (Rep. South Africa).

5) 'The oxidation of alkenes and alkanes by ruthenium tetraoxide - a DFT investigation', November 2005, Symposium Graduate School GK352, TU Berlin (Germany).

6) "Hydrosilylation of carbonyl compounds by metal-oxo catalysis: Manifold mechanisms - a DFT study", September 2007, GdCh Meeting 2007, University Ulm (Germany).