

## List of Publications

Prof. Dr. Walter Thiel

- (1) W. Thiel, F. Weller, J. Lorberth und K. Dehnicke, Z. Anorg. Allg. Chem. **381**, 57-70 (1971).  
Tris(Methylquecksilber)amin und verwandte Verbindungen.
- (2) W. Thiel und A. Schweig, Chem. Phys. Lett. **12**, 49-52 (1971).  
Photoionization Cross Sections in the Valence Electron Approximation. I. Linear Molecules.
- (3) W. Thiel und A. Schweig, Chem. Phys. Lett. **16**, 409-413 (1972).  
Photoionization Cross Sections in the Valence Electron Approximation. II. Relative Intensities in the HeI Photoelectron Spectra of Linear Molecules.
- (4) P. Dechant, A. Schweig und W. Thiel, Angew. Chem. **85**, 358-359 (1973); Angew. Chem., Int. Ed. Engl. **12**, 308-309 (1973).  
Unterschiedliche relative Bandenintensitäten in HeI und HeII Photoelektronenspektren.
- (5) A. Schweig und W. Thiel, J. Electron Spectrosc. **2**, 199-200 (1973).  
Photoionization Cross Sections: HeI and HeII Photoelectron Spectra of Fluorine Compounds.
- (6) A. Schweig und W. Thiel, Chem. Phys. Lett. **21**, 541-543 (1973).  
Photoionization Cross Sections: HeI and HeII Photoelectron Spectra of Saturated Three-Membered Rings.
- (7) A. Schweig und W. Thiel, J. Chem. Phys. **60**, 951-957 (1974).  
Photoionization Cross Sections in the Valence Electron Approximation. III. Nonlinear Molecules (Theory).
- (8) A. Schweig und W. Thiel, Mol. Phys. **27**, 265-268 (1974).  
Photoionization Cross Sections: HeI and HeII Photoelectron Spectra of Homologous Oxygen and Sulphur Compounds.

- (9) A. Schweig und W. Thiel, *J. Electron Spectrosc.* **3**, 27-38 (1974).  
Photoionization Cross Sections: Interpretation of Band Intensities in HeI and HeII Photoelectron Spectra.
- (10) M. J. S. Dewar, A. Komornicki, W. Thiel und A. Schweig, *Chem. Phys. Lett.* **31**, 286-290 (1975).  
Calculation of Photoionization Cross Sections Using Ab initio Wavefunctions and the Plane Wave Approximation.
- (11) M. J. S. Dewar und W. Thiel, *J. Am. Chem. Soc.* **97**, 3978-3986 (1975).  
Ground States of Molecules. XXX. MINDO/3 Study of Reactions of Singlet ( $^1\Delta_g$ ) Oxygen with Carbon–Carbon Double Bonds.
- (12) M. J. S. Dewar, A. C. Griffin, W. Thiel und I. J. Turchi, *J. Am. Chem. Soc.* **97**, 4439-4440 (1975).  
A Possible Mechanism for the Formation of Oxiranes in Reactions of Singlet Molecular Oxygen with Olefins.
- (13) M. J. S. Dewar, R. C. Haddon, W. K. Li, W. Thiel und P. K. Weiner, *J. Am. Chem. Soc.* **97**, 4540-4545 (1975).  
Ground States of Molecules. XXXI. MINDO/3 Study of  $\text{CH}_2$ ,  $\text{NH}_2^+$ , and  $\text{O}_2$ .
- (14) M. J. S. Dewar und W. Thiel, *J. Am. Chem. Soc.* **99**, 2338-2339 (1977).  
MINDO/3 Study of the Addition of Singlet Oxygen ( $^1\Delta_g\text{O}_2$ ) to 1,3-Butadiene.
- (15) M. J. S. Dewar und W. Thiel, *Theor. Chim. Acta* **46**, 89-104 (1977).  
A Semiempirical Model for the Two-Center Repulsion Integrals in the NDDO Approximation.
- (16) M. J. S. Dewar und W. Thiel, *J. Am. Chem. Soc.* **99**, 4899-4907 (1977).  
Ground States of Molecules. 38. The MNDO Method. Approximations and Parameters.
- (17) M. J. S. Dewar und W. Thiel, *J. Am. Chem. Soc.* **99**, 4907-4917 (1977).  
Ground States of Molecules. 39. MNDO Results for Molecules Containing Hydrogen, Carbon, Nitrogen and Oxygen.

- (18) M. J. S. Dewar, G. P. Ford, M. L. McKee, H. S. Rzepa, W. Thiel und Y. Yamaguchi, *J. Mol. Struct.* **43**, 135-138 (1978).  
Semiempirical Calculations of Molecular Frequencies: The MNDO Method.
- (19) H. Schmidt, A. Schweig, W. Thiel und M. Jones, Jr., *Chem. Ber.* **111**, 1958-1961 (1978).  
Photoelektronenspektren und MNDO-Rechnungen für [n]-Paracyclophane.
- (20) H. L. Hase, G. Lauer, K.-W. Schulte, A. Schweig und W. Thiel, *Chem. Phys. Lett.* **54**, 494-497 (1978).  
Calculated Photoelectron Spectra of Singlet and Triplet Methylene.
- (21) V. Eck, G. Lauer, A. Schweig, W. Thiel und H. Vermeer, *Z. Naturforsch., A: Phys., Phys. Chem., Kosmophys.* **33**, 383-385 (1978).  
Preparation and Investigation of Cyclopentadienone by Variable Temperature Photoelectron Spectroscopy.
- (22) A. Schweig und W. Thiel, *Tetrahedron Lett.* 1841-1844 (1978).  
Theoretical Study of Complexes of Cyclobutadiene with Carbonmonoxide and Carbon-dioxide.
- (23) W. Thiel, *Theor. Chim. Acta* **48**, 357-359 (1978).  
The Most Stable CNDO/2 Water Dimer.
- (24) W. Thiel, *QCPE* **11**, 353 (1978).  
MNDO: Molecular Orbital Calculations by the MNDO Method with Geometry Optimization.
- (25) G. Lauer, K.-W. Schulte, A. Schweig und W. Thiel, *Theor. Chim. Acta* **52**, 319-328 (1979).  
Geometry Optimizations with Explicit Inclusion of Electron Correlation.
- (26) H. Woyнар, H. Schäfer, A. Berndt, W. Thiel und A. Schweig, *Z. Naturforsch., B: Anorg. Chem., Org. Chem.* **34**, 1339-1340 (1979).  
Konformationen sterisch gehinderter Anilin-Kationradikale und Benzyl-Kationen.
- (27) A. Schweig und W. Thiel, *J. Am. Chem. Soc.* **101**, 4742-4743 (1979).  
MNDO Study of Tetra-*tert*-butyltetrahedrane and Tetra-*tert*-butylcyclobutadiene and of Their Thermal Interconversion.

- (28) C. Müller, A. Schweig, W. Thiel, W. Grahn, R. G. Bergman und K. P. C. Vollhardt, *J. Am. Chem. Soc.* **101**, 5579-5581 (1979).  
The Photoelectron Spectra of 2,5-Dehydrotropylidene, 3,6-Dehydrooxepin, and Fulvenallene.
- (29) A. Schweig und W. Thiel, *J. Comput. Chem.* **1**, 129-133 (1980).  
The C<sub>4</sub>H<sub>4</sub>CO Potential Surface. Reactions Involving Bicyclo[2.1.0]pentenone.
- (30) W. Thiel, *J. Chem. Soc., Faraday Trans. 2* **76**, 302-308 (1980).  
Multipole Analysis of MNDO Results.
- (31) A. Kos, D. Poppinger, P. v. R. Schleyer und W. Thiel, *Tetrahedron Lett.* 2151-2154 (1980).  
C<sub>2</sub>Li<sub>6</sub> Structural Isomers.
- (32) W. Thiel, *J. Am. Chem. Soc.* **103**, 1413-1420 (1981).  
The MNDOC Method, a Correlated Version of the MNDO Model.
- (33) W. Thiel, *J. Am. Chem. Soc.* **103**, 1420-1425 (1981).  
MNDOC Study of Reactive Intermediates and Transition States.
- (34) A. Schweig und W. Thiel, *J. Am. Chem. Soc.* **103**, 1425-1431 (1981).  
MNDOC Study of Excited States.
- (35) W. Thiel, *Theor. Chim. Acta* **59**, 191-208 (1981).  
Semiempirical NDDO Calculations with STO-3G and 4-31G Basis Sets.
- (36) W. Thiel, *Chem. Phys.* **57**, 227-243 (1981).  
A Comparative Theoretical Study of Photoionization Cross Sections and Angular Distributions.
- (37) J. Kreile, A. Schweig und W. Thiel, *Chem. Phys. Lett.* **79**, 547-552 (1981).  
Experimental and Theoretical Investigation of the Photoionization of Acetylene.
- (38) W. Thiel, P. Weiner, J. Stewart und M. J. S. Dewar, *QCPE* **13**, 428 (1981); *QCPE Bull.* **1**, 73-74 (1981).  
MNDO: Modified Neglect of Diatomic Overlap.

- (39) W. Thiel, Chem. Phys. Lett. **87**, 249-253 (1982).  
Qualitative Interpretation of Photoelectron Angular Distributions of Linear Molecules.
- (40) J. Kreile, A. Schweig und W. Thiel, Chem. Phys. Lett. **87**, 473-476 (1982).  
Experimental and Theoretical Investigation of the Photoionization of Hydrogen Cyanide.
- (41) G. Boche, H. Etzrodt, M. Marsch und W. Thiel, Angew. Chem. **94**, 141 (1982);  
Angew. Chem., Int. Ed. Engl. **21**, 132-133 (1982); Angew. Chem. Suppl. 345-354  
(1982).  
Das Dianion 1,2-Diphenylbenzocyclobutadiendiid.
- (42) G. Boche, H. Etzrodt, M. Marsch und W. Thiel, Angew. Chem. **94**, 141-142 (1982);  
Angew. Chem., Int. Ed. Engl. **21**, 133 (1982); Angew. Chem. Suppl. 355-360 (1982).  
Das Dianion 1,2,3,4-Tetraphenylcyclobutadiendiid.
- (43) G. Boche, R. Eiben und W. Thiel, Angew. Chem. **94**, 703-704 (1982); Angew. Chem.,  
Int. Ed. Engl. **21**, 688-689 (1982); Angew. Chem. Suppl. 1535-1544 (1982).  
Leichte Rotation um die Kohlenstoff-Kohlenstoff-Bindung in Lithium-  
cyclopentadienyl(ester)enolaten.
- (44) G. Boche, F. Heidenhain, W. Thiel und R. Eiben, Chem. Ber. **115**, 3167-3190 (1982).  
Aromatizität als Funktion des Ionenpaarcharakters: Akzeptor-substituierte Cyclonona-  
tetraenyl-Anionen, Enolat-Anionen mit variablen Ladungsverteilungen und ungewöhn-  
lichen konformativen Eigenschaften.
- (45) W. Thiel, QCPE **14**, 438 (1982); QCPE Bull. **2**, 63 (1982).  
MNDOC: Correlated Semiempirical Calculations with Geometry Optimization.
- (46) W. Thiel, J. Electron Spectrosc. Relat. Phenom. **31**, 151-160 (1983).  
Characterization of Resonances in Photoionization.
- (47) W. Thiel, Chem. Phys. **77**, 103-122 (1983).  
Theoretical Analysis of Photoelectron Angular Distributions of Linear Molecules.
- (48) J. Kreile, A. Schweig und W. Thiel, Chem. Phys. Lett. **100**, 351-357 (1983).  
Shape Resonances in the Valence-Shell Photoionization of Cyanogen.

- (49) J. Kreile, A. Schweig und W. Thiel, Chem. Phys. Lett. **108**, 259-265 (1984).  
Shape Resonances in Photoionization: Correlation with STO-3G MO Results.
- (50) W. Thiel, J. Electron Spectrosc. Relat. Phenom. **34**, 399-405 (1984).  
Theoretical Analysis of Photoelectron Angular Distributions in Hydrogen Chloride.
- (51) S. Schröder und W. Thiel, J. Am. Chem. Soc. **107**, 4422-4430 (1985).  
Comparison of Semiempirical and ab Initio Transition States.
- (52) E. A. Halevi und W. Thiel, J. Photochem. **28**, 373-381 (1985).  
The Reactive Excited State of Naphthalene and its Photochemistry: A Qualitative and Quantitative Theoretical Investigation.
- (53) M. G. Hicks und W. Thiel, J. Comput. Chem. **7**, 213-218 (1986).  
Reference Energies in Semiempirical Parametrizations.
- (54) S. Schröder und W. Thiel, J. Mol. Struct.: THEOCHEM **138**, 141-150 (1986).  
Comparison of Semiempirical and ab Initio Transition States for Organic Reactions.
- (55) S. Schröder und W. Thiel, J. Am. Chem. Soc. **108**, 7985-7989 (1986).  
Correlation Effects on Semiempirical Transition States.
- (56) D. Cremer und W. Thiel, J. Comput. Chem. **8**, 48-50 (1987).  
On the Importance of Size-Consistency Corrections in Semiempirical MNDOC Calculations.
- (57) W. Schneider und W. Thiel, J. Chem. Phys. **86**, 923-936 (1987).  
Ab Initio Calculation of Harmonic Force Fields and Vibrational Spectra for the Methyl, Silyl, Germyl, and Stannyl Halides.
- (58) J. Breidung und W. Thiel, J. Phys. Chem. **92**, 5597-5602 (1988).  
Ab Initio Calculation of Harmonic Force Fields and Vibrational Spectra for the Fluorophosphines  $\text{PH}_n\text{F}_{3-n}$  ( $n=0-3$ ).
- (59) J. Breidung, W. Thiel und A. Komornicki, J. Phys. Chem. **92**, 5603-5611 (1988).  
Ab Initio Calculation of Harmonic Force Fields and Vibrational Spectra for the Fluorophosphoranes  $\text{PH}_n\text{F}_{5-n}$  ( $n=0-5$ ).

- (60) W. Schneider, W. Thiel und A. Komornicki, *J. Phys. Chem.* **92**, 5611-5619 (1988).  
Ab Initio Calculation of Harmonic Force Fields and Vibrational Spectra for the Phosphine Oxides and Sulfides  $R_3PY$  ( $R=H,F,CH_3$ ;  $Y=O,S$ ).
- (61) W. Thiel, *J. Mol. Struct.: THEOCHEM* **163**, 415-429 (1988).  
Fast Semiempirical Geometry Optimizations.
- (62) W. Thiel, *Tetrahedron* **44**, 7393-7408 (1988).  
Semiempirical Methods: Current Status and Perspectives.
- (63) D. Higgins, C. Thomson und W. Thiel, *J. Comput. Chem.* **9**, 702-707 (1988).  
Comparison of Semiempirical MO Methods for Open-Shell Systems.
- (64) W. Thiel, G. Scuseria, H. F. Schaefer und W. D. Allen, *J. Chem. Phys.* **89**, 4965-4975 (1988).  
The Anharmonic Force Fields of HOF and  $F_2O$ .
- (65) W. Thiel, H. F. Schaefer und Y. Yamaguchi, *J. Mol. Spectrosc.* **132**, 193-206 (1988).  
The Anharmonic Force Fields of Silyl Fluoride and Silyl Chloride.
- (66) J. Breidung, W. Thiel und A. Komornicki, *Chem. Phys. Lett.* **153**, 76-81 (1988).  
Analytical Second Derivatives for Effective Core Potentials.
- (67) W. Schneider und W. Thiel, *Chem. Phys. Lett.* **157**, 367-373 (1989).  
Anharmonic Force Fields from Analytical Second Derivatives: Method and Application to Methyl Bromide.
- (68) W. Thiel, *Mol. Phys.* **68**, 427-432 (1989).  
Nonlinear Transformation of Anharmonic Normal Coordinate Force Constants.
- (69) W. Schneider, W. Thiel und A. Komornicki, *J. Phys. Chem.* **94**, 2810-2814 (1990).  
Ab Initio Calculation of Harmonic Force Fields and Vibrational Spectra for the Arsine Oxides and Sulfides  $R_3AsY$  ( $R=H,F$ ;  $Y=O,S$ ) and Related Compounds.
- (70) J. Breidung, W. Schneider, W. Thiel und H. F. Schaefer, *J. Mol. Spectrosc.* **140**, 226-236 (1990).  
The Anharmonic Force Fields of  $PH_3$ ,  $PHF_2$ ,  $PF_3$ ,  $PH_5$ , and  $H_3PO$ .

- (71) H. Beckers, J. Breidung, H. Bürger, R. Kuna, A. Rahner, W. Schneider und W. Thiel, *J. Chem. Phys.* **93**, 4603-4614 (1990).  
High-Resolution Rotation-Vibration Spectroscopy of Difluorophosphorane: A Combined Experimental and Theoretical Study.
- (72) J. Breidung, W. Thiel und A. Komornicki, *Inorg. Chem.* **30**, 1067-1073 (1991).  
Ab Initio Calculation of Harmonic Force Fields and Vibrational Spectra of the Fluoroarsines  $\text{AsH}_n\text{F}_{3-n}$  ( $n = 0-3$ ) and the Fluoroarsoranes  $\text{AsH}_n\text{F}_{5-n}$  ( $n = 0-5$ ).
- (73) D. Bakowies und W. Thiel, *J. Am. Chem. Soc.* **113**, 3704-3714 (1991).  
MNDO Study of Large Carbon Clusters.
- (74) D. Bakowies und W. Thiel, *Chem. Phys.* **151**, 309-321 (1991).  
Theoretical Infrared Spectra of Large Carbon Clusters.
- (75) C. Kaupert, H. Heydtmann und W. Thiel, *Chem. Phys.* **156**, 85-93 (1991).  
The Vibrational Spectra of Monohalogenated Cyclopropanes: Ab Initio Calculations and an Experimental Study of Fluorocyclopropane.
- (76) H. Bürger, W. Schneider, S. Sommer, W. Thiel und H. Willner, *J. Chem. Phys.* **95**, 5660-5669 (1991).  
The Vibrational Spectrum and Rotational Constants of Difluoroethyne: Matrix and High Resolution Infrared Studies and Ab Initio Calculations.
- (77) W. Thiel und A. A. Voityuk, *Theor. Chim. Acta* **81**, 391-404 (1992); **93**, 315 (1996).  
Extension of the MNDO Formalism to d Orbitals: Integral Approximations and Preliminary Numerical Results.
- (78) Z. Slanina, L. Adamowicz, D. Bakowies und W. Thiel, *Thermochim. Acta* **202**, 249-254 (1992).  
Fullerene  $\text{C}_{50}$  Isomers: Temperature-Induced Interchange of Relative Stabilities.
- (79) J. Breidung und W. Thiel, *J. Comput. Chem.* **13**, 165-176 (1992).  
A Systematic Ab Initio Study of the Group V Trihalides  $\text{MX}_3$  and Pentahalides  $\text{MX}_5$  ( $\text{M}=\text{P-Bi}$ ,  $\text{X}=\text{F-I}$ ).
- (80) W. Schneider und W. Thiel, *Chem. Phys.* **159**, 49-66 (1992).  
Ab Initio Calculation of Anharmonic Force Fields for the Methyl, Silyl, Germyl, and Stannyl Halides.



- (81) R. Krömer und W. Thiel, *Chem. Phys. Lett.* **189**, 105-111 (1992).  
Ab Initio Calculation of Harmonic Force Fields and Vibrational Spectra for Trichloromethyltitanium and Related Compounds.
- (82) H. Bürger, R. Kuna, G. Pawelke, S. Sommer und W. Thiel, *Z. Naturforsch., A: Phys. Sci.* **47**, 475-479 (1992).  
High Resolution FTIR Study of the  $\nu_8$  Band and Ab Initio Calculation of the Harmonic and Anharmonic Force Field of Difluoromethanimine  $\text{CF}_2\text{NH}$ .
- (83) T. Arthen-Engeland, T. Bultmann, N. P. Ernsting, M. A. Rodriguez und W. Thiel, *Chem. Phys.* **163**, 43-53 (1992).  
Singlet Excited-State Intramolecular Proton Transfer in 2-(2'-Hydroxyphenyl)benzoxazole: Spectroscopy at Low Temperatures, Femtosecond Transient Absorption, and MNDO Calculations.
- (84) W. Thiel und A. A. Voityuk, *Int. J. Quantum Chem.* **44**, 807-829 (1992).  
Extension of MNDO to d Orbitals: Parameters and Results for the Halogens.
- (85) C. Kippels, W. Thiel, D. C. McKean und A. M. Coats, *Spectrochim. Acta, Part A* **48**, 1067-1082 (1992).  
The Harmonic Force Fields of Dimethyl Zinc, Cadmium and Mercury: A Joint Theoretical and Experimental Study.
- (86) D. Bakowies und W. Thiel, *Chem. Phys. Lett.* **192**, 236-242 (1992).  
Theoretical Study of Buckminsterfullerene Derivatives  $\text{C}_{60}\text{X}_n$  ( $\text{X} = \text{H}, \text{F}; n = 2, 36, 60$ ).
- (87) J. Breidung, W. Schneider, W. Thiel und T. J. Lee, *J. Chem. Phys.* **97**, 3498-3499 (1992).  
The Vibrational Frequencies of Difluoroethyne.
- (88) N. P. Ernsting, T. Arthen-Engeland, M. A. Rodriguez und W. Thiel, *J. Chem. Phys.* **97**, 3914-3919 (1992).  
State-Selectivity of Excited-State Intramolecular Proton Transfer in a "Double" Benzoxazole: Jet Spectroscopy and MNDO Calculations.
- (89) D. Bakowies, A. Gelessus und W. Thiel, *Chem. Phys. Lett.* **197**, 324-329 (1992).  
Quantum-Chemical Study of  $\text{C}_{78}$  Fullerene Isomers.

- (90) M. Brumm, G. Frenking, J. Breidung und W. Thiel, *Chem. Phys. Lett.* **197**, 330-334 (1992).  
Large Discrepancies between the Theoretically Predicted and Experimentally Observed Vibrational Frequencies of  $\text{ONCl}_2^+$  and  $\text{ONClF}^+$ .
- (91) D. Bakowies, M. Kolb, W. Thiel, S. Richard, R. Ahlrichs und M. M. Kappes, *Chem. Phys. Lett.* **200**, 411-417 (1992).  
Quantumchemical Study of  $\text{C}_{84}$  Fullerene Isomers.
- (92) M. Kolb und W. Thiel, *J. Comput. Chem.* **14**, 37-44 (1993).  
MNDO Parameters for Helium: Optimization, Tests, and Application to Endohedral Fullerene-Helium Complexes.
- (93) Z. Slanina, J. P. Francois, D. Bakowies und W. Thiel, *J. Mol. Struct.* **279**, 213-216 (1993).  
Fullerene  $\text{C}_{78}$  Isomers: Temperature Dependence of Their Calculated Relative Stabilities.
- (94) T. A. Hein, W. Thiel und T. J. Lee, *J. Phys. Chem.* **97**, 4381-4385 (1993).  
Ab Initio Study of the Stability and Vibrational Spectra of Plumbane, Methylplumbane, and Homologous Compounds.
- (95) M. Kolb und W. Thiel, *J. Comput. Chem.* **14**, 775-789 (1993).  
Beyond the MNDO Model: Methodical Considerations and Numerical Results.
- (96) Z. Slanina, J. P. François, M. Kolb, D. Bakowies und W. Thiel, *Fullerene Sci. Technol.* **1**, 221-230 (1993).  
Calculated Relative Stabilities of  $\text{C}_{84}$ .
- (97) R. Hoos, A. B. Naughton, W. Thiel, A. Vasella, W. Weber, K. Rupitz und S. G. Withers, *Helv. Chim. Acta* **76**, 2666-2686 (1993).  
D-Gluconhydroximo-1,5-lactam and Related N-Arylcarbammates. Theoretical Calculations, Structure, Synthesis, and Inhibitory Effect on  $\beta$ -Glucosidases.
- (98) C. Heinemann und W. Thiel, *Chem. Phys. Lett.* **217**, 11-16 (1994).  
Ab Initio Study on the Stability of Diaminocarbenes.

- (99) A. Vasella, P. Ermert, R. Hoos, A. B. Naughton, K. Rupitz, W. Thiel, M. Weber, W. Weber und S. G. Withers, in: *Complex Carbohydrates in Drug Research*, K. Bock und H. Clausen (Hrsg.), Munksgaard, Kopenhagen, 1994, S. 134-150.  
Synthesis and Evaluation of New Glycosidase Inhibitors.
- (100) J. Breidung und W. Thiel, *J. Mol. Struct.* **320**, 39-47 (1994).  
Theoretical Study of the Harmonic and Anharmonic Force Fields of Phosphorus Pentafluoride.
- (101) W. Thiel und A. A. Voityuk, *J. Mol. Struct.* **313**, 141-154 (1994).  
Extension of MNDO to d Orbitals: Parameters and Results for Silicon.
- (102) C. Heinemann, W. A. Herrmann und W. Thiel, *J. Organomet. Chem.* **475**, 73-84 (1994).  
Theoretical Study of Stable Silylenes and Germynes.
- (103) H. Bürger, R. Kuna, S. Ma, J. Breidung und W. Thiel, *J. Chem. Phys.* **101**, 1-14 (1994).  
The Vibrational Spectra of Krypton and Xenon Difluoride: High Resolution Infrared Studies and Ab Initio Calculations.
- (104) M. Bühl, W. Thiel, H. Jiao, P. v. R. Schleyer, M. Saunders und F. A. L. Anet, *J. Am. Chem. Soc.* **116**, 6005-6006 (1994).  
Helium and Lithium NMR Chemical Shifts of Endohedral Fullerene Compounds: An Ab Initio Study.
- (105) H. Beckers, H. Bürger, R. Kuna, M. Paplewski und W. Thiel, *J. Chem. Phys.* **101**, 5585-5595 (1994).  
Ab Initio Calculations on Monohalogenophosphanes  $\text{PH}_2\text{X}$  ( $\text{X} = \text{F}, \text{Cl}, \text{Br}, \text{I}$ ), and Experimental Detection and Characterization of  $\text{PH}_2\text{F}$  and  $\text{PH}_2\text{Cl}$  by High Resolution Infrared Spectroscopy.
- (106) W. Thiel, *Chimia* **48**, 447-448 (1994).  
Recent Theoretical Fullerene Research.
- (107) M. Bühl, W. Thiel, U. Fleischer und W. Kutzelnigg, *J. Phys. Chem.* **99**, 4000-4007 (1995).  
Ab Initio Computation of  $^{77}\text{Se}$  NMR Chemical Shifts with the IGLO-SCF, the GIAO-SCF, and the GIAO-MP2 Methods.

- (108) J. Breidung und W. Thiel, *J. Mol. Spectrosc.* **169**, 166-180 (1995).  
The Anharmonic Force Fields of Arsine, Stibine, and Bismutine.
- (109) A. M. Coats, D. C. McKean, C. Starcke und W. Thiel, *Spectrochim. Acta, Part A* **51**, 685-697 (1995).  
Experimental and Theoretical Infrared Intensities of the Fundamental Bands of Zinc, Cadmium and Mercury Dimethyls; Electro-Optical Parameters, Atomic Polar Tensors and Effective Atomic Charges.
- (110) J. Breidung, H. Bürger, M. Senzlober und W. Thiel, *Ber. Bunsen-Ges.* **99**, 282-288 (1995).  
The Vibrational Spectrum of Fluorochloroethyne FCCl: Ab Initio Calculations and High Resolution Studies.
- (111) A. Gelessus und W. Thiel, *Ber. Bunsen-Ges.* **99**, 514-519 (1995).  
Theoretical Approaches to Anharmonic Resonances.
- (112) M. Bühl und W. Thiel, *Chem. Phys. Lett.* **233**, 585-589 (1995).  
Ab Initio Helium NMR Chemical Shifts of Endohedral Fullerene Compounds He@C<sub>n</sub> (n = 32-180).
- (113) M. Bühl, W. Thiel und U. Schneider, *J. Am. Chem. Soc.* **117**, 4623-4627 (1995).  
Magnetic Properties of C<sub>60</sub>H<sub>36</sub> Isomers.
- (114) V. Jonas und W. Thiel, *J. Chem. Phys.* **102**, 8474-8484 (1995).  
Theoretical Study of the Vibrational Spectra of the Transition Metal Carbonyls M(CO)<sub>6</sub> [M = Cr, Mo, W], M(CO)<sub>5</sub> [M = Fe, Ru, Os], and M(CO)<sub>4</sub> [M = Ni, Pd, Pt].
- (115) H. Fleischer, D. Hnyk, D. W. H. Rankin, H. E. Robertson, M. Bühl und W. Thiel, *Chem. Ber.* **128**, 807-815 (1995).  
The Molecular Structures and Conformations of Bis(dichlorosilyl)amine and Bis(dichlorosilyl)methylamine in the Gas Phase: Determination by Electron Diffraction and by ab Initio Calculations.
- (116) A. Gelessus, W. Thiel und W. Weber, *J. Chem. Educ.* **72**, 505-508 (1995).  
Multipoles and Symmetry.

- (117) D. Bakowies, M. Bühl und W. Thiel, *J. Am. Chem. Soc.* **117**, 10113-10118 (1995).  
Can Large Fullerenes Be Spherical?
- (118) D. Bakowies, M. Bühl und W. Thiel, *Chem. Phys. Lett.* **247**, 491-493 (1995).  
A Density Functional Study on the Shape of C<sub>180</sub> and C<sub>240</sub> Fullerenes.
- (119) D. G. Green, I. E. Boston und W. Thiel, in: *Lecture Notes in Computer Science*, Bd. 919, B. Hertzberger und G. Serazzi (Hrsg.), Springer-Verlag, Berlin, 1995, S. 880-885.  
Parallelization in Quantum Chemistry: The MNDO Code.
- (120) W. Thiel und D. G. Green, in: *Methods and Techniques in Computational Chemistry*, METECC-95, E. Clementi und G. Corongiu (Hrsg.), STEF-Verlag, Cagliari, 1995, S. 141-168.  
The MNDO94 Code: Parallelization of a Semiempirical Quantum-chemical Program.
- (121) W. Thiel, *Adv. Chem. Phys.* **93**, 703-757 (1996).  
Perspectives on Semiempirical Molecular Orbital Theory.
- (122) J. Cioslowski, S. Patchkovskii und W. Thiel, *Chem. Phys. Lett.* **248**, 116-120 (1996).  
Electronic Structures, Geometries, and Energetics of Highly Charged Cations of the C<sub>60</sub> Fullerene.
- (123) D. Bakowies und W. Thiel, *J. Comput. Chem.* **17**, 87-108 (1996).  
Semiempirical Treatment of Electrostatic Potentials and Partial Atomic Charges in Combined Quantum Chemical and Molecular Mechanical Approaches.
- (124) W. Thiel und A. A. Voityuk, *J. Phys. Chem.* **100**, 616-626 (1996).  
Extension of MNDO to d Orbitals: Parameters and Results for the Second-Row Elements and for the Zinc Group.
- (125) S. Patchkovskii und W. Thiel, *Theor. Chim. Acta* **93**, 87-99 (1996).  
Analytical First Derivatives of the Energy in the MNDO Half-Electron Open-Shell Treatment.
- (126) S. Patchkovskii und W. Thiel, *J. Comput. Chem.* **17**, 1318-1327 (1996).  
Analytical Second Derivatives of the Energy in MNDO Methods.

- (127) H. Bürger, S. Ma, J. Breidung und W. Thiel, *J. Chem. Phys.* **104**, 4945-4953 (1996).  
*Ab Initio* Calculations and High Resolution Infrared Investigation on XeF<sub>4</sub>.
- (128) M. Malagoli und W. Thiel, *Chem. Phys.* **206**, 73-85 (1996).  
A Semiempirical Approach to Nonlinear Optical Properties of Large Molecules at the MNDO and MNDO/d Level.
- (129) D. Bakowies und W. Thiel, *J. Phys. Chem.* **100**, 10580-10594 (1996).  
Hybrid Models for Combined Quantum Mechanical and Molecular Mechanical Approaches.
- (130) S. Bailleux, M. Bogey, J. Breidung, H. Bürger, R. Fajgar, Y. Liu, J. Pola, M. Senzlober und W. Thiel, *Angew. Chem.* **108**, 2683-2685 (1996); *Angew. Chem., Int. Ed. Engl.* **35**, 2513-2515 (1996).  
Silaethene H<sub>2</sub>C=SiH<sub>2</sub>: Millimeter Wave Spectrum and *Ab Initio* Calculations.
- (131) J. Breidung, T. Hansen und W. Thiel, *J. Mol. Spectrosc.* **179**, 73-78 (1996).  
Equilibrium Structure and Spectroscopic Constants of Difluoroethyne: An *Ab Initio* Study.
- (132) V. Jonas und W. Thiel, *J. Chem. Phys.* **105**, 3636-3648 (1996).  
Theoretical Study of the Vibrational Spectra of the Transition Metal Hydrides HM(CO)<sub>5</sub> [M = Mn, Re], H<sub>2</sub>M(CO)<sub>4</sub> [M = Fe, Ru, Os], and HM(CO)<sub>4</sub> [M = Co, Rh, Ir].
- (133) S. Patchkovskii und W. Thiel, *J. Am. Chem. Soc.* **118**, 7164-7172 (1996).  
How Does Helium Get Into Buckminsterfullerene?
- (134) D. Bakowies, M. Bühl, S. Patchkovskii und W. Thiel, in: *Fullerenes: Recent Advances in the Physics and Chemistry of Fullerenes and Related Materials*, Bd. 3, R. S. Ruoff und K. M. Kadish (Hrsg.), The Electrochemical Society, Pennington, NJ, 1996, S. 901-910.  
Theoretical Studies on Giant Fullerenes and on Endohedral Fullerene Complexes.
- (135) P. Dréan, M. Paplewski, J. Demaison, J. Breidung, W. Thiel, H. Beckers und H. Bürger, *Inorg. Chem.* **35**, 7671-7678 (1996).  
Millimeterwave Spectra, *ab Initio* Calculations, and Structures of Fluorophosphane and Chlorophosphane.

- (136) S. Patchkovskii und W. Thiel, *J. Chem. Phys.* **106**, 1796-1799 (1997).  
Equilibrium Yield for Helium Incorporation into Buckminsterfullerene: Quantum-chemical Evaluation.
- (137) J. Breidung, W. Thiel und J. Demaison, *Chem. Phys. Lett.* **266**, 515-520 (1997).  
Equilibrium Structure of PH<sub>2</sub>Br.
- (138) G. S. McGrady, A. J. Downs, N. C. Bednall, D. C. McKean, W. Thiel, V. Jonas, G. Frenking und W. Scherer, *J. Phys. Chem. A* **101**, 1951-1968 (1997).  
Infrared Spectrum and Structure of Me<sub>2</sub>TiCl<sub>2</sub> and Quantum Mechanical Calculations of Geometries and Force Fields for MeTiCl<sub>3</sub> and Me<sub>2</sub>TiCl<sub>2</sub>.
- (139) F. Cardullo, P. Seiler, L. Isaacs, J.-F. Nierengarten, R. F. Haldimann, F. Diederich, T. Mordasini-Denti, W. Thiel, C. Boudon, J.-P. Gisselbrecht und M. Gross, *Helv. Chim. Acta* **80**, 343-371 (1997).  
Bis- through Tetrakis-Adducts of C<sub>60</sub> by Reversible Tether-directed Remote Functionalization and Systematic Investigation of the Changes in Fullerene Properties as a Function of Degree, Pattern, and Nature of Functionalization.
- (140) S. Patchkovskii und W. Thiel, *Helv. Chim. Acta* **80**, 495-509 (1997).  
Radical Impurity Mechanisms for Helium Incorporation into Buckminsterfullerene.
- (141) M. Filatov und W. Thiel, *Int. J. Quantum Chem.* **62**, 603-616 (1997).  
A Nonlocal Correlation Energy Density Functional from a Coulomb Hole Model.
- (142) M. Filatov und W. Thiel, *Mol. Phys.* **91**, 847-859 (1997).  
A New Gradient-Corrected Exchange-Correlation Density Functional.
- (143) J. Heyd, W. Thiel und W. Weber, *J. Mol. Struct.* **391**, 125-130 (1997).  
Rotation and Inversion Barriers in N-Methylmethanesulfonamide from Ab Initio Calculations.
- (144) H. Bürger, P. Weinrath, S. Dressler, T. Hansen und W. Thiel, *J. Mol. Spectrosc.* **183**, 139-150 (1997).  
High Resolution Infrared Studies and Quantum-Chemical Calculations on MnO<sub>3</sub>F.

- (145) H. Bürger und W. Thiel, in: *Vibration-Rotational Spectroscopy and Molecular Dynamics*, D. Papousek (Hrsg.), World Scientific, Singapore, 1997, S. 56-115.  
Vibration-Rotation Spectra of Reactive Molecules: Interplay of Ab Initio Calculations and High-Resolution Experimental Studies.
- (146) W. Thiel, *J. Mol. Struct.* **398**, 1-6 (1997).  
Computational Methods for Large Molecules.
- (147) M. Bühl und W. Thiel, *Inorg. Chem.* **36**, 2922-2924 (1997).  
A Density Functional Study of the Rotational Barrier of Tricarbonyl ( $\eta^4$ -norbornadiene)iron. Effect of the Torsional Angle on the Carbonyl Stretching Spectra.
- (148) S. Bailleux, M. Bogey, J. Demaison, H. Bürger, M. Senzlober, J. Breidung, W. Thiel, R. Fajgar und J. Pola, *J. Chem. Phys.* **106**, 10016-10026 (1997).  
The Equilibrium Structure of Silene  $\text{H}_2\text{C}=\text{SiH}_2$  from Millimeter Wave Spectra and from Ab Initio Calculations.
- (149) J. Breidung, H. Bürger, C. Kötting, R. Kopitzky, W. Sander, M. Senzlober, W. Thiel und H. Willner, *Angew. Chem.* **109**, 2072-2075 (1997); *Angew. Chem., Int. Ed. Engl.* **36**, 1983-1985 (1997).  
Difluorovinyliden  $\text{F}_2\text{C}=\text{C}$ .
- (150) J. Breidung und W. Thiel, *J. Mol. Spectrosc.* **185**, 115-122 (1997).  
Equilibrium Structure and Spectroscopic Constants of Dichloroethyne: An ab Initio Study.
- (151) S. Dressler und W. Thiel, *Chem. Phys. Lett.* **273**, 71-78 (1997).  
Anharmonic Force Fields from Density Functional Theory.
- (152) S. Patchkovskii und W. Thiel, *Theor. Chem. Acc.* **98**, 1-4 (1997).  
Analytical First Derivatives of the Energy for Small CI Expansions.
- (153) M. Bühl, S. Patchkovskii und W. Thiel, *Chem. Phys. Lett.* **275**, 14-18 (1997).  
Interaction Energies and NMR Chemical Shifts of Noble Gases in  $\text{C}_{60}$ .
- (154) J. Barluenga, J. M. Gonzalez, I. Llorente, P. J. Campos, M. A. Rodriguez und W. Thiel, *J. Organomet. Chem.* **548**, 185-189 (1997).  
Theoretical Evidence for Stereoselective Lithiations of 2-Alkoxy-1,1-diiodo-1-alkenes. An ab Initio Study.



- (155) C. Boudon, J.-P. Gisselbrecht, M. Gross, F. Cardullo, P. Seiler, L. Isaacs, J.-F. Nierengarten, R. Haldimann, F. Diederich, T. Mordasini-Denti und W. Thiel, in: Fullerenes: Recent Advances in the Physics and Chemistry of Fullerenes and Related Materials, Bd. 5, R. S. Ruoff und K. M. Kadish (Hrsg.), The Electrochemical Society, Pennington, NJ, 1997, S. 95-98.  
Redox Behavior of Mono- Through Hexakis-Adducts of C<sub>60</sub> Fullerenes.
- (156) S. Patchkovskii und W. Thiel, in: Fullerenes: Recent Advances in the Physics and Chemistry of Fullerenes and Related Materials, Bd. 5, R. S. Ruoff und K. M. Kadish (Hrsg.), The Electrochemical Society, Pennington, NJ, 1997, S. 126-137.  
Theoretical Studies of Helium Incorporation by Buckminsterfullerene.
- (157) W. Thiel, in: Computational Thermochemistry, K. K. Irikura und D. J. Frurip (Hrsg.), ACS Symposium Series 677, American Chemical Society, Washington, DC, 1998, S. 142-161.  
Thermochemistry from Semiempirical Molecular Orbital Theory.
- (158) M. Filatov und W. Thiel, Phys. Rev. A: At., Mol., Opt. Phys. **57**, 189-199 (1998).  
Exchange-Correlation Density Functional Beyond the Gradient Approximation.
- (159) V. Jonas und W. Thiel, Organometallics **17**, 353-360 (1998).  
Density Functional Study of the Vibrational Spectra of Octahedral Transition Metal Hexacarbonyls: Neutral Molecules (M = Cr, Mo, W) and Isoelectronic Ions (M = V, Nb, Ta; Mn, Re; Fe, Ru, Os; Co, Rh, Ir; Pt; Au).
- (160) P. T. Brain, M. Bühl, H. E. Robertson, A. D. Jackson, P. D. Lickiss, D. MacKerracher, D. W. H. Rankin, D. Shah und W. Thiel, J. Chem. Soc., Dalton Trans. 545-551 (1998).  
Structures of Ga(hfac)<sub>3</sub> and In(hfac)<sub>3</sub> (hfac = 1,1,1,5,5,5-hexafluoropentane-2,4-dionate) in the Gas Phase as Studied by Electron Diffraction and *ab initio* Calculations.
- (161) H. Fleischer, P. T. Brain, D. W. H. Rankin, H. E. Robertson, M. Bühl und W. Thiel, J. Chem. Soc., Dalton Trans. 593-600 (1998).  
Gas-Phase Molecular Structures of Bis(chloromethylsilyl)amine and Bis(chloromethylsilyl)methylamine by Electron Diffraction and Ab Initio Calculations; Experimental Support for n(N)-σ\*(Si-Cl)-Hyperconjugation.

- (162) W. Thiel, *Nachr. Chem., Tech. Lab.* **46**, 198-201 (1998).  
Embedding.
- (163) C. Kötting, W. Sander, J. Breidung, W. Thiel, M. Senzlober und H. Bürger, *J. Am. Chem. Soc.* **120**, 219-220 (1998).  
A Charge-Transfer Complex of Xenon and Difluorovinylidene.
- (164) S. Patchkovskii und W. Thiel, *J. Am. Chem. Soc.* **120**, 556-563 (1998).  
C<sub>60</sub> Dimers: A Route to Endohedral Fullerene Compounds?
- (165) W. Thiel, in: *Encyclopedia of Computational Chemistry*, P. v. R. Schleyer (Hrsg.), Wiley, Chichester, UK, 1998, S. 1599-1604.  
MNDO.
- (166) W. Thiel, in: *Encyclopedia of Computational Chemistry*, P. v. R. Schleyer (Hrsg.), Wiley, Chichester, UK, 1998, S. 1604-1605.  
MNDO/d.
- (167) I. Antes und W. Thiel, in: *Combined Quantum Mechanical and Molecular Mechanical Methods*, J. Gao und M. A. Thompson (Hrsg.), ACS Symposium Series 712, American Chemical Society, Washington, DC, 1998, S. 50-65.  
On the Treatment of Link Atoms in Hybrid Methods.
- (168) T. Z. Mordasini, C. Hanser und W. Thiel, *Chem. Phys. Lett.* **288**, 183-187 (1998).  
Molecular Structure of the Fullerene C<sub>70</sub> at 825°C: Quantum-chemical Molecular Dynamics Simulations.
- (169) T. Z. Mordasini und W. Thiel, *Chimia* **52**, 288-291 (1998).  
Combined Quantum Mechanical and Molecular Mechanical Approaches.
- (170) M. Rotger, V. Boudon, B. Lavorel, S. Sommer, H. Bürger, J. Breidung, W. Thiel, M. Bétrencourt und J.-C. Deroche, *J. Mol. Spectrosc.* **192**, 294-308 (1998).  
*Ab Initio* Calculations and High-Resolution Spectroscopy of the Bending Pentad of SiH<sub>2</sub>D<sub>2</sub> in the 10-16  $\mu$ m Region.
- (171) J. Breidung und W. Thiel, *Theor. Chem. Acc.* **100**, 183-190 (1998).  
Anharmonic Force Field and Spectroscopic Constants of Silene: An *Ab Initio* Study.

- (172) M. Filatov und W. Thiel, Chem. Phys. Lett. **295**, 467-474 (1998).  
Tests of a Density Functional with Laplacian Terms: Activation Barriers and Bond-Stretching Energies.
- (173) C. Boudon, J.-P. Gisselbrecht, M. Gross, F. Cardullo, P. Seiler, L. Isaacs, J.-F. Nierengarten, R. F. Haldimann, F. Diederich, T. Mordasini-Denti und W. Thiel, Can. J. Chem. Eng. **76**, 1008-1012 (1998).  
Propriétés rédox de fullerènes fonctionnalisés.
- (174) J. Breidung, H. Bürger, D. McNaughton, M. Senzlober und W. Thiel, Spectrochim. Acta, Part A **55**, 695-708 (1999).  
Ab Initio and High Resolution Infrared Study of FCCBr.
- (175) J. Breidung, W. Thiel, J. Gauss und J. F. Stanton, J. Chem. Phys. **110**, 3687-3696 (1999).  
Anharmonic Force Fields from Analytic CCSD(T) Second Derivatives: HOF and F<sub>2</sub>O.
- (176) A. Herrmann, M. W. Rüttimann, T. Gibtner, C. Thilgen, F. Diederich, T. Mordasini und W. Thiel, Helv. Chim. Acta **82**, 261-289 (1999).  
Achiral and Chiral Higher Adducts of C<sub>70</sub> by Bingel Cyclopropanation.
- (177) H. Jacobsen, V. Jonas, D. Werner, A. Messmer, J.-C. Panitz, H. Berke und W. Thiel, Helv. Chim. Acta **82**, 297-307 (1999).  
Vibrational Spectra of Nitrosyl Substituted Transition Metal Hydride Complexes: An Experimental and Theoretical Study of Carbonyldihydronitrosyl (trimethylphosphine)-rhenium Re(CO)H<sub>2</sub>(NO)(PMe<sub>3</sub>)<sub>2</sub>.
- (178) S. Patchkovskii und W. Thiel, J. Comput. Chem. **20**, 1220-1245 (1999).  
NMR Chemical Shifts in MNDO Approximation: Parameters and Results for H, C, N, and O.
- (179) A. J. Lupinetti, V. Jonas, W. Thiel, S. H. Strauss und G. Frenking, Chem. Eur. J. **5**, 2573-2583 (1999).  
Trends in Molecular Geometries and Bond Strengths of the Homoleptic d<sup>10</sup> Metal Carbonyl Cations [M(CO)<sub>n</sub>]<sup>x+</sup> (M<sup>x+</sup> = Cu<sup>+</sup>, Ag<sup>+</sup>, Au<sup>+</sup>, Zn<sup>2+</sup>, Cd<sup>2+</sup>, Hg<sup>2+</sup>; n = 1-6).  
A Theoretical Study.

- (180) V. Jonas und W. Thiel, J. Phys. Chem. A **103**, 1381-1393 (1999).  
Symmetry Force Fields for Neutral and Ionic Transition Metal Carbonyl Complexes from Density Functional Theory.
- (181) J. Demaison, J. Breidung, W. Thiel und D. Papousek, Struct. Chem. **10**, 129-133 (1999).  
The Equilibrium Structure of Methyl Fluoride.
- (182) M. T. Reetz, E. Bohres, R. Goddard, M. C. Holthausen und W. Thiel, Chem. Eur. J. **5**, 2101-2108 (1999).  
Synthesis, Solid State Structure and Electronic Nature of a Phosphinine-Stabilized *triangulo* Palladium Cluster.
- (183) J. Breidung, H. Bürger, M. Senzlober und W. Thiel, Z. Naturforsch., A: Phys. Sci. **54**, 236-244 (1999).  
High Resolution FTIR Spectrum of Chlorofluoroethyne, FCCl, below 1000 cm<sup>-1</sup>. Analysis of the  $\nu_3$ ,  $\nu_4$ ,  $\nu_5$ ,  $2\nu_4$ ,  $\nu_4+\nu_5$  and  $2\nu_5$  bands, and ab initio Calculations.
- (184) X. Daura, I. Antes, W. F. van Gunsteren, W. Thiel und A. E. Mark, Proteins: Struct., Funct., Genet. **36**, 542-555 (1999).  
The Effect of Motional Averaging on the Calculation of NMR Structural Properties.
- (185) M. Senzlober, H. Bürger, R. Eujen, A. Gelessus und W. Thiel, J. Fluorine Chem. **99**, 99-104 (1999).  
Squaric Acid Difluoride.
- (186) H. Beckers, J. Breidung, H. Bürger, R. Köppe, C. Kötting, W. Sander, H. Schnöckel und W. Thiel, Eur. J. Inorg. Chem. 2013-2019 (1999).  
Difluorosilanethione F<sub>2</sub>Si = S by Flash Vacuum Thermolysis of (F<sub>3</sub>Si)<sub>2</sub>S and by Reaction of SiS with F<sub>2</sub> – Matrix Studies and Ab Initio Calculations.
- (187) J. C. W. Lohrenz, M. Bühl, M. Weber und W. Thiel, J. Organomet. Chem. **592**, 11-21 (1999).  
A Density Functional Study on the Formation of Stereoerrors in the Stereoselective Propene Polymerization with Zirconocene Catalysts.
- (188) I. Antes und W. Thiel, J. Phys. Chem. A **103**, 9290-9295 (1999).  
Adjusted Connection Atoms for Combined Quantum Mechanical and Molecular Mechanical Methods.

- (189) J. Demaison, L. Margulès, J. Breidung, W. Thiel und H. Bürger, *Mol. Phys.* **97**, 1053-1067 (1999).  
*Ab Initio* Anharmonic Force Field, Spectroscopic Parameters, and Equilibrium Structure of Trifluorosilane.
- (190) V. Jonas und W. Thiel, *J. Chem. Soc., Dalton Trans.* 3783-3790 (1999).  
Theoretical Study on Linear Dicyanide und Dicarbonyl Complexes of the Metals Au, Hg, and Tl: On the Possible Existence of a  $[\text{Tl}(\text{CO})_2]^{3+}$  Cation.
- (191) J. Breidung, J. Demaison, L. Margulès und W. Thiel, *Chem. Phys. Lett.* **313**, 713-717 (1999).  
Equilibrium Structure of  $\text{SiF}_4$ .
- (192) E. Bernhardt, H. Willner, V. Jonas, W. Thiel und F. Aubke, *Angew. Chem.* **112**, 173-176 (2000); *Angew. Chem., Int. Ed.* **39**, 168-171 (2000).  
Das Tetrakis(carbonyl)dioxoosmium (VI)-Kation: *trans*- $[\text{OsO}_2(\text{CO})_4]^{2+}$ .
- (193) W. Weber und W. Thiel, *Theor. Chem. Acc.* **103**, 495-506 (2000).  
Orthogonalization Corrections for Semiempirical Methods.
- (194) J. Breidung und W. Thiel, *Z. Allg. Anorg. Chem.* **626**, 362-367 (2000).  
Equilibrium Structure and Fundamental Vibrational Wavenumbers in Difluorosilanone: An *ab Initio* Study.
- (195) H. Willner, C. Bach, R. Wartchow, C. Wang, S. J. Rettig, J. Trotter, V. Jonas, W. Thiel und F. Aubke, *Inorg. Chem.* **39**, 1933-1942 (2000).  
Syntheses, Molecular Structures, and Vibrational Spectra of Chloropentacarbonylrhodium(III) and -iridium(III) Undecafluorodiantimonate(V),  $[\text{Rh}(\text{CO})_5\text{Cl}][\text{Sb}_2\text{F}_{11}]_2$  and  $[\text{Ir}(\text{CO})_5\text{Cl}][\text{Sb}_2\text{F}_{11}]_2$ : An Experimental and Density Functional Study.
- (196) S. Patchkovskii und W. Thiel, *J. Mol. Model.* **6**, 67-75 (2000).  
Nucleus-Independent Chemical Shifts from Semiempirical Calculations.
- (197) W. Thiel, in: *Modern Methods and Algorithms in Quantum Chemistry*, J. Grotendorst (Hrsg.), NIC Series, Bd. 1, Jülich, 2000, S. 233-255.  
Semiempirical Methods.

- (198) S. R. Billeter, A. J. Turner und W. Thiel, *Phys. Chem. Chem. Phys.* **2**, 2177-2186 (2000).  
Linear Scaling Geometry Optimisation and Transition State Search in Hybrid Delocalized Internal Coordinates.
- (199) H. Beckers, M. Bogey, J. Breidung, H. Bürger, P. Dréan, P. Papelewski, W. Thiel und A. Walters, *Phys. Chem. Chem. Phys.* **2**, 2467-2469 (2000).  
FP=S in the Gas Phase: Detection by Rotationally-Resolved Infrared and Millimeter-Wave Spectra Assisted by Ab Initio Calculations.
- (200) Z. Chen, H. Jiao, A. Hirsch und W. Thiel, *Chem. Phys. Lett.* **329**, 47-51 (2000).  
Fullerenes  $C_{36}^n$  ( $n = 0, 2+, 2-$ ) and their B- and N-doped analogues.
- (201) C. D. Berweger, W. Thiel und W. F. van Gunsteren, *Proteins: Struct., Funct., Genet.* **41**, 299-315 (2000).  
Molecular-Dynamics Simulation of the  $\beta$  Domain of Metallothionein With a Semi-Empirical Treatment of the Metal Core.
- (202) J. Breidung und W. Thiel, *J. Mol. Spectrosc.* **205**, 28-37 (2001).  
Equilibrium Structure and Spectroscopic Constants of Difluorvinylidene: An Ab Initio Study.
- (203) J. Breidung und W. Thiel, *J. Mol. Struct.* **599**, 239-254 (2001).  
Equilibrium Structure and Fundamental Vibrational Wavenumbers in Monomeric Methylithium  $CH_3Li$ : An Ab Initio Study.
- (204) F. A. Hamprecht, C. Peter, X. Daura, W. Thiel und W. F. van Gunsteren, *J. Chem. Phys.* **114**, 2079-2089 (2001).  
A Strategy for Analysis of (Molecular) Equilibrium Simulations: Configuration Space Density Estimation, Clustering and Visualization.
- (205) H. Willner, M. Bodenbinder, R. Bröchler, G. Hwang, S. J. Rettig, J. Trotter, B. von Ahsen, U. Westphal, V. Jonas, W. Thiel und F. Aubke, *J. Am. Chem. Soc.* **123**, 588-602 (2001).  
Superelectrophilic Tetrakis(carbonyl)palladium(II)- and -platinum(II) Undecafluoro-diantimonate(V),  $[Pd(CO)_4][Sb_2F_{11}]_2$  and  $[Pt(CO)_4][Sb_2F_{11}]_2$ : Syntheses, Physical and Spectroscopic Properties, Their Crystal, Molecular, and Extended Structures, and Density Functional Calculations: An Experimental, Computational, and Comparative Study.

- (206) A. Döhring, V. R. Jensen, P. W. Jolly, W. Thiel und J. C. Weber, *Organometallics* **20**, 2234-2245 (2001).  
Donor-Ligand-Substituted Cyclopentadienylchromium(III) Complexes: A New Class of Alkene Polymerization Catalyst. 2. Phosphinoalkyl-Substituted Systems.
- (207) H. Bürger, M. Lecoutre, T. R. Huet, J. Breidung, W. Thiel, V. Hänninen und L. Halonen, *J. Chem. Phys.* **114**, 8844-8854 (2001).  
The  $(n00)$ ,  $n = 3, 4$ , and 6, Local Mode States of  $H_3SiD$ : Fourier Transform Infrared and Laser Photoacoustic Spectra and Ab Initio Calculations of Spectroscopic Parameters.
- (208) K. Möhle, H.-J. Hofmann und W. Thiel, *J. Comput. Chem.* **22**, 509-520 (2001).  
Description of Peptide and Protein Secondary Structures Employing Semiempirical Methods.
- (209) A. Döhring, V. R. Jensen, P. W. Jolly, W. Thiel und J. C. Weber, in: *Organometallic Catalysts and Olefin Polymerization*, R. Blom, A. Follestad, E. Rytter, M. Tilset und M. Ystenes (Hrsg.), Springer-Verlag, Berlin, 2001, S. 127-136.  
Phosphinoalkyl-Substituted Cyclopentadienyl Chromium Catalysts for the Oligomerization of Ethylene.
- (210) A. Döhring, V. R. Jensen, P. W. Jolly, W. Thiel und J. C. Weber, *Macromol. Symp.* **173**, 117-121 (2001).  
Steric Control of the Chromium-Catalyzed Oligomerization of Ethylene.
- (211) Z. Chen, H. Jiao, A. Hirsch und W. Thiel, *J. Mol. Model.* **7**, 161-163 (2001).  
The  $2(N+1)^2$  Rule for Spherical Aromaticity: Further Validation.
- (212) S. R. Billeter, C. F. W. Hanser, T. Z. Mordasini, M. Scholten, W. Thiel und W. F. van Gunsteren, *Phys. Chem. Chem. Phys.* **3**, 688-695 (2001).  
Molecular Dynamics Study of Oxygenation Reactions Catalysed by the Enzyme p-Hydroxybenzoate Hydroxylase.
- (213) Z. Chen, H. Jiao, A. Hirsch und W. Thiel, *J. Org. Chem.* **66**, 3380-3383 (2001).  
BN-doped Fullerenes: A NICS Characterization.
- (214) W. Thiel, in: *Quantum-Mechanical Prediction of Thermochemical Data*, J. Cioslowski (Hrsg.), Kluwer Academic, Dordrecht, 2001, S. 235-245.  
Semiempirical Thermochemistry: A Brief Survey.

- (215) H. Lin, H. Bürger, S.-G. He, L.-F. Yuan, J. Breidung und W. Thiel, *J. Phys. Chem. A* **105**, 6065-6072 (2001).  
Overtones of the Si-H Stretching-Bending Polyad in SiHD<sub>3</sub>: Internal Coordinate Force Field, *Ab Initio* Dipole Moment Surfaces, and Band Intensities.
- (216) H. Lin, H. Bürger, E. B. MKadmi, S.-G. He, L.-F. Yuan, J. Breidung, W. Thiel, T. R. Huet und J. Demaison, *J. Chem. Phys.* **115**, 1378-1391 (2001).  
The Si-H Stretching-Bending Overtone Polyads of SiHF<sub>3</sub>: Assignments, Band Intensities, Internal Coordinate Force Field, and *Ab Initio* Dipole Moment Surfaces.
- (217) H. Lin, S.-G. He, X.-G. Wang, L.-F. Yuan, H. Bürger, J.-F. D'Eu, N. Reuter und W. Thiel, *Phys. Chem. Chem. Phys.* **3**, 3506-3517 (2001).  
The Vibrational Overtones of SiH<sub>4</sub> Isotopomers: Experimental Wavenumbers, Assignment, *Ab Initio* Dipole Moment Surfaces, and Intensities.
- (218) Z. Chen, H. Jiao, M. Bühl, A. Hirsch und W. Thiel, *Theor. Chem. Acc.* **106**, 352-363 (2001).  
Theoretical Investigation into Structures and Magnetic Properties of Smaller Fullerenes and their Heteroanalogues.
- (219) Z. Chen, J. Cioslowski, N. Rao, D. Moncrieff, M. Bühl, A. Hirsch und W. Thiel, *Theor. Chem. Acc.* **106**, 364-368 (2001).  
Endohedral Chemical Shifts in Higher Fullerenes with 72-86 Carbon Atoms.
- (220) Z. Chen, U. Reuther, A. Hirsch und W. Thiel, *J. Phys. Chem. A* **105**, 8105-8110 (2001).  
Theoretical Studies on the Substitution Patterns in Heterofullerenes C<sub>70-x</sub>N<sub>x</sub> and C<sub>70-x</sub>B<sub>x</sub> ( $x = 2-10$ ).
- (221) H. Beckers, H. Bürger, P. Papelewski, M. Bogey, J. Demaison, P. Dréan, A. Walters, J. Breidung und W. Thiel, *Phys. Chem. Chem. Phys.* **3**, 4247-4257 (2001).  
Millimeter-Wave Spectroscopy, High Resolution Infrared Spectrum, *Ab Initio* Calculations, and Molecular Geometry of FPO.
- (222) F. A. Hamprecht, U. Achleitner, A. C. Krismer, K. H. Lindner, V. Wenzel, H.-U. Strohmenger, W. Thiel, W. F. van Gunsteren und A. Amann, *Resuscitation* **50**, 287-296 (2001).  
Fibrillation Power, an Alternative Method of ECG Spectral Analysis for Prediction of Countershock Success in a Porcine Model of Ventricular Fibrillation.



- (223) V. R. Jensen und W. Thiel, *Organometallics* **20**, 4852-4862 (2001).  
Computational Investigation of Ethylene Insertion into the Metal-Methyl Bond of First-Row Transition Metal(III) Species.
- (224) G. Fink, R. A. Wendt, K. Angermund, V. R. Jensen und W. Thiel, *Polym. Mater.: Sci. Eng.* **84**, 255-256 (2001).  
Metallocene/MAO Catalyzed Polymerizations of Functionalized Norbornene Derivatives: Copolymerizations Using Ethene, and Terpolymerizations Using Ethene and Norbornene.
- (225) S.-G. He, H. Lin, W. Thiel und Q.-S. Zhu, *Chem. Phys. Lett.* **349**, 131-136 (2001).  
Four-Dimensional Dipole Moment Surfaces and Local Mode Vibrational Band Intensities of GeH<sub>4</sub>.
- (226) H. Beckers, M. Bogey, J. Breidung, H. Bürger, J. Demaison, P. Dréan, P. Paplewski, W. Thiel und A. Walters, *J. Mol. Spectrosc.* **210**, 213-223 (2001).  
Millimeter-Wave Spectroscopy, High Resolution Infrared Spectrum, *Ab Initio* Calculations, and Molecular Geometry of FPS.
- (227) S.-G. He, H. Lin, H. Bürger, W. Thiel, Y. Ding und Q.-S. Zhu, *J. Chem. Phys.* **116**, 105-111 (2002).  
Calculation of the Si-H Stretching-Bending Overtones in SiHCl<sub>3</sub> Employing *Ab Initio* Potential Energy and Dipole Moment Surfaces
- (228) C. Lennartz, A. Schäfer, F. Terstegen und W. Thiel, *J. Phys. Chem. B* **106**, 1758-1767 (2002).  
Enzymatic Reactions of Triosephosphate Isomerase: A Theoretical Calibration Study.
- (229) F. A. Hamprecht, W. Thiel und W. F. van Gunsteren, *J. Chem. Inf. Comput. Sci.* **42**, 414-428 (2002).  
Chemical Library Subset Selection Algorithms: A Unified Derivation Using Spatial Statistics.
- (230) M. N. Jagadeesh, W. Thiel, J. Köhler und A. Fehn, *Organometallics* **21**, 2076-2087 (2002).  
Hydrosilylation with bis(alkynyl)(1,5-cyclooctadiene)platinum catalysts: A density functional study of the initial activation.

- (231) N. Reuter, H. Lin und W. Thiel, *J. Phys. Chem. B* **106**, 6310-6321 (2002).  
Green Fluorescent Proteins: Empirical force field for the neutral and deprotonated forms of the chromophore. Molecular dynamics simulations of the wild type and S65T mutant.
- (232) J. C. Schöneboom, H. Lin, N. Reuter, W. Thiel, S. Cohen, F. Ogliaro und S. Shaik, *J. Am. Chem. Soc.* **124**, 8142-8151 (2002).  
The Elusive Oxidant Species of Cytochrome P450 Enzymes: Characterization by Combined Quantum Mechanical/ Molecular Mechanical (QM/MM) Calculations.
- (233) W. Jerzembeck, H. Bürger, L. Constantin, L. Margulès, J. Demaison, J. Breidung und W. Thiel, *Angew. Chem.* **114**, 2659-2661 (2002); *Angew. Chem., Int. Ed.* **41**, 2550-2552 (2002).  
Bismuthine BiH<sub>3</sub>: Fact or Fiction? High Resolution Infrared, Millimeter-Wave and Ab Initio Studies.
- (234) S. F. Vyboishchikov, M. Bühl und W. Thiel, *Chem. Eur. J.* **8**, 3962-3975 (2002).  
Mechanism of Olefin Metathesis Catalyzed by Ruthenium Carbene Complexes: Density Functional Studies on Model Systems.
- (235) H. Jiao, Z. Chen, A. Hirsch und W. Thiel, *Phys. Chem. Chem. Phys.* **4**, 4916-4920 (2002).  
Oxa- and Thia-Fullerenes (C<sub>59</sub>O, C<sub>59</sub>S): Closed or Opened Cages?
- (236) I. Antes, W. Thiel und W. F. van Gunsteren, *Eur. Biophys. J.* **31**, 504-520 (2002).  
Molecular Dynamics Simulations of Photoactive Yellow Protein (PYP) in Three States of its Photocycle: A Comparison with X-ray and NMR Data and Analysis of the Effects of Glu46 Deprotonation and Mutation.
- (237) J. Breidung und W. Thiel, *J. Mol. Spectrosc.* **216**, 424-427 (2002).  
Ab Initio Study of the Charge-Transfer Complex of Xenon and Dicarbon.
- (238) H. Lin, W. Thiel, S. N. Yurchenko, M. Carvajal und P. Jensen, *J. Chem. Phys.* **117**, 11265-11276 (2002).  
Vibrational Energies for NH<sub>3</sub> Based on High Level Ab Initio Potential Energy Surfaces.

- (239) W. Thiel, in : Jahrbuch 2002 der Max-Planck-Gesellschaft, Verlag Vandenhoeck & Ruprecht, Göttingen, 2002, S. 509-516.  
Untersuchungen zur übergangsmetallkatalysierten Olefinpolymerisation und zur Modellierung enzymatischer Reaktionen.
- (240) Z. Chen und W. Thiel, Chem. Phys. Lett. **367**, 15-25 (2003).  
Performance of Semiempirical Methods in Fullerene Chemistry: Relative Energies and Nucleus-Independent Chemical Shifts.
- (241) Z. Chen, W. Thiel und A. Hirsch, Chem. Phys. Chem. **4**, 93-97 (2003).  
Reactivity of the Convex and Concave Surfaces of Single-Walled Carbon Nanotubes (SWCNTs) towards Addition Reactions: Dependence on the Carbon-Atom Pyramidalization.
- (242) Z. Zelinger, P. Dréan, A. Walters, J. R. A. Moreno, M. Bogey, H. Pernice, S. von Ahsen, H. Willner, J. Breidung, W. Thiel und H. Bürger, J. Chem. Phys. **118**, 1214-1220 (2003).  
Gas-Phase Detection of the FCO<sub>2</sub> Radical by Millimeter Wave and High Resolution Infrared Spectroscopy Assisted by Ab Initio Calculations.
- (243) W. Thiel, in: Handbook of Molecular Physics and Quantum Chemistry, Bd. 2, S. Wilson (Hrsg.), Wiley, Chichester, 2003, S. 487-502.  
Semiempirical Theories.
- (244) E. Bernhardt, H. Willner, A. Kornath, J. Breidung, M. Bühl, V. Jonas und W. Thiel, J. Phys. Chem. A **107**, 859-868 (2003).  
D<sub>3d</sub> Ground-State Structure of V(CO)<sub>6</sub>: A Combined Matrix Isolation and Ab Initio Study of the Jahn-Teller Effect.
- (245) Z. Chen, H. Jiao, D. Moran, A. Hirsch, W. Thiel und P. v. R. Schleyer, J. Phys. Chem. A **107**, 2075-2079 (2003).  
Structures and Stabilities of Endo- and Exohedral Dodecahedrane Complexes (X@C<sub>20</sub>H<sub>20</sub> and XC<sub>20</sub>H<sub>20</sub>, X=H<sup>+</sup>, H, N, P, C<sup>-</sup>, Si<sup>-</sup>, O<sup>+</sup>, S<sup>+</sup>).
- (246) H. Jiao, Z. Chen, A. Hirsch und W. Thiel, J. Mol. Model. **9**, 34-38 (2003).  
Structures and Magnetic Properties of Mono-Doped Fullerenes C<sub>59</sub>X<sup>n</sup> and C<sub>59</sub>X<sup>(6-n)-</sup> (X = B<sup>-</sup>, N<sup>+</sup>, P<sup>+</sup>, As<sup>+</sup>, Si) : Isoelectronic Analogues of C<sub>60</sub> and C<sub>60</sub><sup>6-</sup>.

- (247) Z. Chen, H. Jiao, G. Seifert, A. H. C. Horn, D. Yu, T. Clark, W. Thiel und P. v. R. Schleyer, *J. Comput. Chem.* **24**, 948-953 (2003).  
The Structure and Stability of Si<sub>60</sub> and Ge<sub>60</sub> Cages: A Computational Study.
- (248) C. E. Taylor, M. G. Cory, R. J. Bartlett und W. Thiel, *Comput. Mater. Sci.* **27**, 204-211 (2003).  
The Transfer Hamiltonian: A Tool for Large Scale Simulations with Quantum Mechanical Forces.
- (249) A. Kosłowski, M. E. Beck und W. Thiel, *J. Comput. Chem.* **24**, 714-726 (2003).  
Implementation of a General Multireference Configuration Interaction Procedure with Analytic Gradients in a Semiempirical Context Using the Graphical Unitary Group Approach.
- (250) J. Breidung, L. Constantin, J. Demaison, L. Margulès und W. Thiel, *Mol. Phys.* **101**, 1113-1122 (2003).  
Ground State Rotational Spectrum,  $K = 3$  Splittings, *Ab Initio* Anharmonic Force Field and Equilibrium Structure of Trifluoroamine.
- (251) T. Sternfeld, C. Thilgen, Z. Chen, S. Siefken, P. v. R. Schleyer, W. Thiel, F. Diederich und M. Rabinovitz, *J. Org. Chem.* **68**, 4850-4854 (2003).  
Fullerene Anions of Different Sizes and Shapes: A <sup>13</sup>C NMR and Density-Functional Study.
- (252) P. Sherwood, A. H. de Vries, M. F. Guest, G. Schreckenbach, C. R. A. Catlow, S. A. French, A. A. Sokol, S. T. Bromley, W. Thiel, A. J. Turner, S. Billeter, F. Terstegen, S. Thiel, J. Kendrick, S. C. Rogers, J. Casci, M. Watson, F. King, E. Karlsen, M. Sjøvoll, A. Fahmi, A. Schäfer und C. Lennartz, *J. Mol. Struct.: THEOCHEM* **632**, 1-28 (2003).  
QUASI: A General Purpose Implementation of the QM/MM Approach and its Application to Problems in Catalysis.
- (253) Z. Chen, H. Jiao, D. Moran, A. Hirsch, W. Thiel und P. v. R. Schleyer, *J. Phys. Org. Chem.* **16**, 726-730 (2003).  
Aromatic Stabilization in Heterofullerenes C<sub>48</sub>X<sub>12</sub> (X = N, P, B, Si).
- (254) S. A. Funke, A. Eipper, M. T. Reetz, N. Otte, W. Thiel, G. van Pouderoyen, B. W. Dijkstra, K.-E. Jaeger und T. Eggert, *Biocatal. Biotransform.* **21**, 67-73 (2003).  
Directed Evolution of an Enantioselective *Bacillus Subtilis* Lipase.

- (255) Z. Cao, Z. Zhou, H. Wan, Q. Zhang und W. Thiel, *Inorg. Chem.* **42**, 6986-6988 (2003).  
Density Functional Calculations on the Binding of Dinitrogen to the FeFe Cofactor in Fe-only Nitrogenase: FeFeco( $\mu_6$ -N<sub>2</sub>) as Intermediate in Nitrogen Fixation.
- (256) Z. Chen, L. R. Sutton, D. Moran, A. Hirsch, W. Thiel und P. v. R. Schleyer, *J. Org. Chem.* **68**, 8808-8814 (2003).  
A Theoretical and Structural Investigation of Thiocarbon Anions.
- (257) Z. Chen, A. Hirsch, S. Nagase, W. Thiel und P. v. R. Schleyer, *J. Am. Chem. Soc.* **125**, 15507-15511 (2003).  
Spherical Sila- and Germa-Homoaromaticity.
- (258) S. P. de Visser, S. Shaik, P. K. Sharma, D. Kumar und W. Thiel, *J. Am. Chem. Soc.* **125**, 15779-15788 (2003).  
The Active Species of Horseradish Peroxidase (HRP) and Cytochrome P450: Two Electronic Chameleons.
- (259) M. Bocola, N. Otte, K.-E. Jaeger, M. T. Reetz und W. Thiel, *ChemBioChem* **5**, 214-223 (2004).  
Learning from Directed Evolution: Theoretical Investigations on Cooperative Mutations in Lipase Enantioselectivity.
- (260) Z. Chen, S. Nagase, A. Hirsch, R. C. Haddon, W. Thiel und P. v. R. Schleyer, *Angew. Chem.* **116**, 1578-1580 (2004); *Angew. Chem., Int. Ed.* **43**, 1552-1554 (2004).  
Side-Wall Opening of Single-Wall Carbon Nanotubes (SWCNTs) by Chemical Modification: A Critical Theoretical Study.
- (261) C. Karafilidis, H. Hermann, A. Rufinska, B. Gabor, R. J. Mynott, G. Breitenbruch, C. Weidenthaler, J. Rust, W. Joppek, M. S. Brookhart, W. Thiel und G. Fink, *Angew. Chem.* **116**, 2498-2500 (2004); *Angew. Chem., Int. Ed.* **43**, 2444-2446 (2004).  
Metallocene-Catalyzed C7-Linkage in the Hydrooligomerization of Norbornene via  $\sigma$ -Bond Metathesis: A new Insight into the Microstructure of Polynorbornene.
- (262) R. A. Wendt, K. Angermund, V. Jensen, W. Thiel und G. Fink, *Macromol. Chem. Phys.* **205**, 308-318 (2004).  
Ethene Copolymerization with Trialkylsilyl Protected Polar Norbornene Derivatives.

- (263) Z. Chen, T. Heine, H. Jiao, A. Hirsch, W. Thiel und P. v. R. Schleyer, *Chem. Eur. J.* **10**, 963-970 (2004).  
Theoretical Studies on the Smallest Fullerene: from Monomer to Oligomers and Solid States.
- (264) J. C. Schöneboom, S. Cohen, H. Lin, S. Shaik und W. Thiel, *J. Am. Chem. Soc.* **126**, 4017-4034 (2004).  
QM/MM Investigation of the Mechanism of C–H Hydroxylation of Camphor by Cytochrome P450<sub>cam</sub>: Theory Supports a Two-State Rebound Mechanism.
- (265) J. C. Schöneboom und W. Thiel, *J. Phys. Chem. B* **108**, 7468-7478 (2004).  
The Resting State of P450<sub>cam</sub>: A QM/MM study.
- (266) W. Thiel, *Chimia* **58**, 276-280 (2004).  
Ab Initio Vibration-Rotation Spectroscopy.
- (267) J. Breidung, W. Thiel, D. Figgen und H. Stoll, *J. Chem. Phys.* **120**, 10404-10413 (2004).  
A Systematic Ab Initio Study of The Equilibrium Geometry and Vibrational Wavenumbers of Bismuthine.
- (268) W. Jerzembeck, H. Bürger, J. Breidung und W. Thiel, *J. Mol. Spectrosc.* **226**, 32-44 (2004).  
High Resolution Infrared Spectra of the  $\nu_1$  -  $\nu_4$  Bands of BiH<sub>3</sub> and Ab Initio Calculations of the Spectroscopic Parameters.
- (269) H. Lin, J. C. Schöneboom, S. Cohen, S. Shaik und W. Thiel, *J. Phys. Chem. B* **108**, 10083-10088 (2004).  
QM/MM Study of the Product-Enzyme Complex in P450<sub>cam</sub> Catalysis.
- (270) F. L. Gu, Z. Chen, H. Jiao, W. Q. Tian, Y. Aoki, W. Thiel und P. v. R. Schleyer, *Phys. Chem. Chem. Phys.* **6**, 4566-4570 (2004).  
Study on the Optical and Magnetic Properties of C<sub>48</sub>N<sub>12</sub> Azafullerene Isomers.
- (271) M. Bühl und W. Thiel, *Inorg. Chem.* **43**, 6377-6382 (2004).  
Density Functional Study of Valence Trapping in a Mixed-Valent Dimanganese Complex.

- (272) L. J. Gooßen, D. Koley, H. Hermann und W. Thiel, Chem. Commun. 2141-2143 (2004).  
The Mechanism of the Oxidative Addition of Aryl Halides to Pd-Catalysts: A DFT Investigation.
- (273) T. Häber, R. Kevorkiants, W. Thiel und M. A. Suhm, Phys. Chem. Chem. Phys. **6**, 4939-4949 (2004).  
The Performance of the Semi-Empirical AM1 Method on Small and Nanometer-Sized N<sub>2</sub>O Clusters.
- (274) J. Breidung, J. Demaison, J.-F. D'Eu, L. Margulès, D. Collet, E. B. Mkadmi, A. Perrin und W. Thiel, J. Mol. Spectrosc. **228**, 7-22 (2004).  
Ground State Constants, Ab Initio Anharmonic Force Field and Equilibrium Structure of F<sub>2</sub>BOH.
- (275) X. Lu, Z. Chen, W. Thiel, P. v. R. Schleyer, R. Huang und L. Zheng, J. Am. Chem. Soc. **126**, 14871-14878 (2004).  
Properties of Fullerene[50] and D<sub>5h</sub> Decachlorofullerene[50]: A Computational Study.
- (276) J. Breidung, J. Cosléou, J. Demaison, K. Sarka und W. Thiel, Mol. Phys. **102**, 1827-1841 (2004).  
Ab Initio Anharmonic Force Field, Molecular Parameters, Equilibrium Structure and Heat of Formation of Fluoroform.
- (277) S. N. Yurchenko, M. Carvajal, P. Jensen, H. Lin, J. Zheng und W. Thiel, Mol. Phys. **103**, 359-378 (2005).  
Rotation-Vibration Motion of Pyramidal XY<sub>3</sub> Molecules Described in the Eckart Frame: Theory and Applications to NH<sub>3</sub>.
- (278) A. Altun und W. Thiel, J. Phys. Chem. B **109**, 1268-1280 (2005).  
Combined Quantum Mechanical/Molecular Mechanical Study on the Pentacoordinated Ferric and Ferrous Cytochrome P450<sub>cam</sub> Complexes.
- (279) S. N. Yurchenko, W. Thiel, S. Patchkovskii und P. Jensen, Phys. Chem. Chem. Phys. **7**, 573-582 (2005).  
Theoretical Evidence for the Formation of Rotational Energy Level Clusters in the Vibrational Ground State of PH<sub>3</sub>.

- (280) M. Wanko, M. Hoffmann, P. Strodel, A. Koslowski, W. Thiel, F. Neese, T. Frauenheim und M. Elstner, *J. Phys. Chem. B* **109**, 3606-3615 (2005).  
Calculating Absorption Shifts for Retinal Proteins: Computational Challenges.
- (281) E. Canè, G. Di Lonardo, L. Fusina, W. Jerzembeck, H. Bürger, J. Breidung und W. Thiel, *Mol. Phys.* **103**, 557-577 (2005).  
The Rotation Spectrum and Infrared Fundamental Bands of  $^{123}\text{SbD}_3$ . Determination of the Molecular Geometry, and *Ab Initio* Calculations of Spectroscopic Parameters.
- (282) S. N. Yurchenko, M. Carvajal, H. Lin, J. Zheng, W. Thiel und P. Jensen, *J. Chem. Phys.* **122**, 104317/1-14 (2005).  
Dipole Moment and Rovibrational Intensities in the Electronic Ground State of  $\text{NH}_3$ . Bridging the Gap between *Ab Initio* Theory and Spectroscopic Experiment.
- (283) J. C. Schöneboom, F. Neese und W. Thiel, *J. Am. Chem. Soc.* **127**, 5840-5853 (2005).  
Towards Identification of the Compound I Reactive Intermediate in Cytochrome P450 Chemistry: A QM/MM Study of its EPR and Mössbauer Parameters.
- (284) W. Thiel, in *Theory and Applications of Computational Chemistry: The First 40 Years*, C. E. Dykstra, K. S. Kim, G. Frenking und G. E. Scuseria (Hrsg.), Elsevier, Amsterdam, 2005, S. 559-580.  
Semiempirical Quantum-Chemical Methods in Computational Chemistry.
- (285) L. J. Goossen, D. Koley, H. L. Hermann und W. Thiel, *Organometallics* **24**, 2398-2410 (2005).  
Mechanistic Pathways for Oxidative Addition of Aryl Halides to Palladium (0) Complexes: A DFT Study.
- (286) H. M. Senn, S. Thiel und W. Thiel, *J. Chem. Theory Comput.* **1**, 494-505 (2005).  
Enzymatic Hydroxylation in *p*-Hydroxybenzoate Hydroxylase: A Case Study for QM/MM Molecular Dynamics.
- (287) J. Khandogin, B. A. Gregersen, W. Thiel und D. M. York, *J. Phys. Chem. B* **109**, 9799-9809 (2005).  
Smooth Solvation Method for d-Orbital Semiempirical Calculations of Biological Reactions. 1. Implementation.



- (288) B. A. Gregersen, J. Khandogin, W. Thiel und D. M. York, *J. Phys. Chem. B* **109**, 9810-9817 (2005).  
Smooth Solvation Method for d-Orbital Semiempirical Calculations of Biological Reactions. 2. Application to Transphosphorylation Thio Effects in Solution.
- (289) S. Shaik, D. Kumar, S. P. de Visser, A. Altun und W. Thiel, *Chem. Rev.* **105**, 2279-2328 (2005).  
A Theoretical Perspective on Structure and Mechanism of Cytochrome P450 Enzymes.
- (290) S. F. Vyboishchikov und W. Thiel, *Chem. Eur. J.* **11**, 3921-3935 (2005).  
Ring Closing Olefin Metathesis on Ruthenium Carbene Complexes: Model DFT Study of Stereochemistry.
- (291) S. N. Yurchenko, W. Thiel, M. Carvajal, H. Lin und P. Jensen, *Adv. Quantum Chem.* **48**, 209-238 (2005).  
Rotation-Vibration Motion of Pyramidal  $XY_3$  Molecules Described in the Eckart Frame: The Calculation of Intensities with Application to  $NH_3$ .
- (292) M. T. Reetz, A. Meiswinkel, G. Mehler, K. Angermund, M. Graf, W. Thiel, R. Mynott und D. Blackmond, *J. Am. Chem. Soc.* **127**, 10305-10313 (2005).  
Why are BINOL-Based Monophosphites Such Efficient Ligands in Rh-Catalyzed Asymmetric Olefin-Hydrogenation?
- (293) L. J. Goossen, D. Koley, H. L. Hermann und W. Thiel, *J. Am. Chem. Soc.* **127**, 11102-11114 (2005).  
The Palladium-Catalyzed Cross-Coupling Reaction of Carboxylic Anhydrides with Arylboronic Acids: A DFT Study.
- (294) R. Steiger, C. H. Bischof, B. Lang und W. Thiel, *Future Gener. Comput. Syst.* **21**, 1324-1332 (2005).  
Using Automatic Differentiation to Compute Derivatives for a Quantum-Chemical Computer Program.
- (295) S. Huang, Z. Xiao, F. Wang, J. Zhou, G. Yuan, S. Zhang, Z. Chen, W. Thiel, P. v. R. Schleyer, X. Zhang, X. Hu, B. Chen und L. Gan, *Chem. Eur. J.* **11**, 5449-5456 (2005).  
Preparation of [5,6] and [6,6] Oxa-homofullerene Derivates and their Interconversion through Lewis Acid Assisted Reactions of Fullerene-mixed Peroxides.

- (296) V. R. Jensen, M. Graf und W. Thiel, *ChemPhysChem* **6**, 1929-1933 (2005).  
Unusual Temperature Effects in Propene Polymerisation Using Stereorigid Zirconocene Catalysts.
- (297) H. Hirao, D. Kumar, W. Thiel und S. Shaik, *J. Am. Chem. Soc.* **127**, 13007-13018 (2005).  
Two States and Two More in the Mechanisms of Hydroxylation and Epoxidation by Cytochrome P450.
- (298) S. Patchkovskii, A. Koslowski und W. Thiel, *Theor. Chem. Acc.* **114**, 84-89 (2005).  
Generic Implementation of Analytical CI Gradients for NDDO-Type Methods.
- (299) E. Derat, S. Cohen, S. Shaik, A. Altun und W. Thiel, *J. Am. Chem. Soc.* **127**, 13611-13621 (2005).  
Principal Active Species of Horseradish Peroxidase, Compound I: A Hybrid Quantum Mechanical/Molecular Mechanical Study.
- (300) H. M. Senn, D. O'Hagan und W. Thiel, *J. Am. Chem. Soc.* **127**, 13643-13655 (2005).  
Insight Into Enzymatic C-F Bond Formation from QM and QM/MM Calculations.
- (301) S. N. Yurchenko, J. Zheng, H. Lin, P. Jensen und W. Thiel, *J. Chem. Phys.* **123**, 134308/1-14 (2005).  
Potential Energy Surface for the Electronic Ground State of  $\text{NH}_3$  up to  $20000 \text{ cm}^{-1}$  above Equilibrium.
- (302) J. Kästner und W. Thiel, *J. Chem. Phys.* **123**, 144104/1-5 (2005).  
Bridging the Gap Between Thermodynamic Integration and Umbrella Sampling Provides a Novel Analysis Method: "Umbrella Integration".
- (303) S. N. Yurchenko, J. Breidung und W. Thiel, *Theor. Chem. Acc.* **144**, 333-340 (2005).  
Vibrational Spectrum of  $\text{BiH}_3$ : Six-Dimensional Variational Calculations on High Level *ab Initio* Potential Energy Surfaces.
- (304) S. A. Funcke, N. Otte, T. Eggert, M. Bocola, K.-E. Jaeger und W. Thiel, *Protein Eng., Des. Sel.* **18**, 509-514 (2005).  
Combination of Computational Prescreening and Experimental Library Construction can Accelerate Enzyme Optimization by Directed Evolution.

- (305) D. Kumar, H. Hirao, S. P. de Visser, J. Zheng, D. Wang, W. Thiel und S. Shaik, J. Phys. Chem. B **109**, 19946-19951 (2005).  
New Features in the Catalytic Cycle of Cytochrome P450 During Formation of Compound I from Compound 0.
- (306) V. R. Jensen, D. Koley, M. N. Jagadeesh und W. Thiel, Macromolecules **38**, 10266-10278 (2005).  
DFT Investigation of the Single-Center, Two-State Model for the Broken Rate Order of Transition Metal Catalyzed Olefin Polymerization.
- (307) L. J. Goossen, D. Koley, H. L. Hermann und W. Thiel, Organometallics **25**, 54-67 (2006).  
Palladium Monophosphine Intermediates in Catalytic Cross-Coupling Reactions: A DFT Study.
- (308) W. Raballand, M. Rotger, V. Boudon, M. Loëte, J. Breidung und W. Thiel, J. Mol. Struct. **780**, 70-79 (2006).  
Stark Effect in X<sub>2</sub>Y<sub>4</sub> Molecules: Application to Ethylene.
- (309) E. Canè, G. Di Lonardo, L. Fusina, W. Jerzembeck, H. Bürger, J. Breidung und W. Thiel, J. Mol. Struct. **780**, 98-110 (2006).  
Rotation Spectrum and High Resolution Infrared Spectra of the Fundamental Bands of <sup>121</sup>SbD<sub>3</sub>. Determination of the Ground State and Equilibrium Structures. *Ab Initio* Calculations of the Spectroscopic Parameters.
- (310) A. Fu, B. List und W. Thiel, J. Org. Chem. **71**, 320-326 (2006).  
Mechanism and Origin of Enantioselectivity of the 2-Methylproline-Catalyzed  $\alpha$ -Alkylation of Aldehydes by Density Functional Theory.
- (311) J. Breidung und W. Thiel, J. Phys. Chem. A. **110**, 1575-1585 (2006).  
Thermochemistry of the Fluoroformyloxyl Radical: A Computational Study Based on Coupled Cluster Theory.
- (312) Z. J. Jakubek, P. R. Bunker, M. Zachwieja, S. G. Nakhate, B. Simard, S. N. Yurchenko, W. Thiel und P. Jensen, J. Chem. Phys. **124**, 094306/1-5 (2006).  
A Dispersed Fluorescence and Ab Initio Investigation of the  $\tilde{X}^2B_1$  and  $\tilde{A}^2A_1$  Electronic States of the PH<sub>2</sub> Molecule.

- (313) J. Kästner, H. M. Senn, S. Thiel, N. Otte und W. Thiel, *J. Chem. Theory Comp.* **2**, 452-461 (2006).  
QM/MM Free-Energy Perturbation Compared to Thermodynamic Integration and Umbrella Sampling: Application to an Enzymatic Reaction.
- (314) A. Altun, V. Guallar, R. A. Friesner, S. Shaik und W. Thiel, *J. Am. Chem. Soc.* **128**, 3924-3925 (2006).  
The Effect of Heme Environment on the Hydrogen Abstraction Reaction of Camphor in P450<sub>cam</sub> Catalysis: A QM/MM Study.
- (315) A. Altun, S. Shaik und W. Thiel, *J. Comput. Chem.* **27**, 1324-1337 (2006).  
Systematic QM/MM Investigation of Factors that Affect the Cytochrome P450<sub>cam</sub>-Catalyzed Hydrogen Abstraction of Camphor.
- (316) J. Kästner und W. Thiel, *J. Chem. Phys.* **124**, 234106/1-7 (2006).  
Analysis of the Statistical Error in Umbrella Sampling Simulations by Umbrella Integration.
- (317) A. Fu und W. Thiel, *J. Mol. Struct.: THEOCHEM* **765**, 45-52 (2006).  
Density Functional Study of Noncovalent Catalysis of the Diels-Alder Reaction by the Neutral Hydrogen Bond Donors Thiourea and Urea.
- (318) S. N. Yurchenko, J. Zheng, W. Thiel, M. Carvajal, H. Lin und P. Jensen, in: *Remote Sensing of the Atmosphere for Environment Security*, A. Perrin (Hrsg.), Springer, Dordrecht, 2006, S. 171-183.  
Theoretical Quantitative Spectroscopy: Computer Simulation of Molecular Spectra.
- (319) M. Hoffmann, M. Wanko, P. Strodel, P. H. König, T. Frauenheim, K. Schulten, W. Thiel, E. Tajkhorshid und M. Elstner, *J. Am. Chem. Soc.* **128**, 10808-10818 (2006).  
Color Tuning in Rhodopsins: The Mechanism for the Spectral Shift Between Bacteriorhodopsin and Sensory Rhodopsin II.
- (320) S. N. Yurchenko, M. Carvajal, W. Thiel und P. Jensen, *J. Mol. Spectrosc.* **239**, 71-87 (2006).  
*Ab Initio* Dipole Moment and Theoretical Rovibrational Intensities in the Electronic Ground State of PH<sub>3</sub>.

- (321) T. Tuttle, D. Wang, W. Thiel, J. Köhler, M. Hofmann und J. Weis, *Organometallics* **25**, 4504-4513 (2006).  
Mechanism of Olefin Hydrosilylation Catalyzed by  $\text{RuCl}_2(\text{CO})_2(\text{PPh}_3)_2$  : A DFT Study.
- (322) T. Tuttle, E. Keinan und W. Thiel, *J. Phys. Chem. B* **110**, 19685-19695 (2006).  
Understanding the Enzymatic Activity of 4-Oxalocrotonate Tautomerase and its Mutant Analogs: A Computational Study.
- (323) J. Zheng, D. Wang, W. Thiel und S. Shaik, *J. Am. Chem. Soc.* **128**, 13204-13215 (2006).  
QM/MM Study of Mechanisms for Compound I Formation in the Catalytic Cycle of Cytochrome P450cam.
- (324) M. Graf, K. Angermund, G. Fink, W. Thiel und V. R. Jensen, *J. Organomet. Chem.* **691**, 4367-4378 (2006).  
Site Epimerization in *ansa*-Zirconocene Polymerization Catalysts.
- (325) F. Claeysens, J. N. Harvey, F. R. Manby, R. A. Mata, A. J. Mulholland, K. E. Ranaghan, M. Schütz, S. Thiel, W. Thiel und H.-J. Werner, *Angew. Chem.* **118**, 7010-7013 (2006); *Angew. Chem., Int. Ed.* **45**, 6856-6859 (2006).  
High Accuracy Computation of Reaction Barriers in Enzymes.
- (326) S. N. Yurchenko, W. Thiel, P. Jensen und P. R. Bunker, *J. Mol. Spectrosc.* **239**, 160-173 (2006).  
Rotation-Vibration Energy Level Clustering in the  $\tilde{X}^2B_1$  Ground Electronic State of  $\text{PH}_2$ .
- (327) S. N. Yurchenko, W. Thiel und P. Jensen, *J. Mol. Spectrosc.* **240**, 174-187 (2006).  
Rotational Energy Cluster Formation in  $\text{XY}_3$  Molecules: Excited Vibrational States of  $\text{BiH}_3$  and  $\text{SbH}_3$ .
- (328) A. Fürstner, D. Kirk, M. D. B. Fenster, C. Aïssa, D. De Souza, C. Nevado, C. T. Tuttle, W. Thiel und O. Müller, *Chem. Eur. J.* **13**, 135-149 (2007).  
Latrunculin Analogues with Improved Biological Profiles by "Diverted Total Synthesis": Preparation, Evaluation and Computational Analysis.

- (329) M. T. Reetz, M. Puls, J. D. Carballeira, A. Vogel, K.-E. Jaeger, T. Eggert, W. Thiel, M. Bocola und N. Otte, *ChemBioChem* **8**, 106-112 (2007).  
Learning from Directed Evolution: Further Lessons from Theoretical Investigations into Cooperative Mutations in Lipase Enantioselectivity.
- (330) H. M. Senn und W. Thiel, in: *Atomistic Approaches in Modern Biology*, M. Reiher (Hrsg.), *Topics in Current Chemistry*, Bd. 268, Springer, Berlin, 2007, S. 173-290.  
QM/MM Methods for Biological Systems.
- (331) M. Mladenovic, T. Schirmeister, S. Thiel, W. Thiel und B. Engels, *ChemMedChem* **2**, 120-128 (2007).  
About the Importance of the Active Site Histidine for the Activity of Epoxide or Aziridine Based Inhibitors of Cysteine Proteases.
- (332) H. M. Senn und W. Thiel, *Curr. Opin. Chem. Biol.* **11**, 182-187 (2007).  
QM/MM Studies of Enzymes.
- (333) T. Tuttle, D. Wang, W. Thiel, J. Köhler, M. Hofmann und J. Weis, *J. Organomet. Chem.* **692**, 2282-2290 (2007).  
Mechanism of Olefin Hydrosilylation Catalyzed by  $[\text{RuCl}(\text{NCCH}_3)_5]^+$ : A DFT Study.
- (334) C. Karafilidis, K. Angermund, B. Gabor, A. Ruffinska, R. J. Mynott, G. Breitenbruch, W. Thiel und G. Fink, *Angew. Chem.* **119**, 3819-3823 (2007); *Angew. Chem., Int. Ed.* **46**, 3745-3749 (2007).  
Helical Microstructure of Polynorbornene.
- (335) J. Kästner, S. Thiel, H. M. Senn, P. Sherwood und W. Thiel, *J. Chem. Theory Comp.* **3**, 1064-1072 (2007).  
Exploiting QM/MM Capabilities in Geometry Optimization: A Microiterative Approach Using Electrostatic Embedding.
- (336) M. P. Waller, M. Bühl, K. R. Geethalakshmi, D. Wang und W. Thiel, *Chem. Eur. J.* **13**, 4723-4732 (2007).  
 $^{51}\text{V}$  NMR Chemical Shifts Calculated from QM/MM Models of Vanadium Chloroperoxidase.
- (337) W. Thiel, in: *Molecular Quantum Mechanics: Analytic Gradients and Beyond*, A. G. Csaszar, G. Fogarasi, H. F. Schaefer und P. G. Szalay (Hrsg.), ELTE Institute of Chemistry, Budapest, 2007, S. 119-121.  
Fast Semiempirical Calculations.

- (338) T. Tuttle und W. Thiel, *J. Phys. Chem. B* **111**, 7665-7674 (2007).  
Substrate Orientation in 4-Oxalocrotonate Tautomerase and its Effect on QM/MM Energy Profiles.
- (339) N. Otte, M. Scholten und W. Thiel, *J. Phys. Chem. A* **111**, 5751-5755 (2007).  
Looking at Self-Consistent-Charge Density Functional Tight Binding from a Semiempirical Perspective.
- (340) D. A. Jose, P. Kar, D. Koley, B. Ganguly, W. Thiel, G. Ramakrishna, D. K. Palit, H. N. Ghosh und A. Das, *Inorg. Chem.* **46**, 5576-5584 (2007).  
Phenol and Catechol-Based Ruthenium(II) Polypyridyl Complexes as Colorimetric Sensors for Fluoride Ion.
- (341) B. Ganguly, D. Koley und W. Thiel, *Tetrahedron* **63**, 7970-7976 (2007).  
Intra-annular Cyclophane Diamines as Proton Sponges: A Computational Study.
- (342) D. P. Geerke, S. Thiel, W. Thiel und W. F. van Gunsteren, *J. Chem. Theory Comp.* **3**, 1499-1509 (2007).  
Combined QM/MM Molecular Dynamics Study on a Condensed-Phase S<sub>N</sub>2 Reaction at Nitrogen: The Effect of Explicitly Including Solvent Polarization.
- (343) T. Tuttle, E. Kraka, W. Thiel und D. Cremer, *J. Phys. Chem. B* **111**, 8321-8328 (2007).  
A QM/MM Study of the Bergman Reaction of Dynemicin A in the Minor Groove of DNA.
- (344) J. Zheng, A. Altun und W. Thiel, *J. Comput. Chem.* **28**, 2147-2158 (2007).  
Common System Setup for the Entire Catalytic Cycle of Cytochrome P450<sub>cam</sub> in Quantum Mechanical/Molecular Mechanical Studies.
- (345) A. Altun, S. Shaik und W. Thiel, *J. Am. Chem. Soc.* **129**, 8978-8987 (2007).  
What is the Active Species of Cytochrome P450 during Camphor Hydroxylation? QM/MM Studies of Different Electronic States of Compound I and of Reduced and Oxidized Iron-Oxo Intermediates.
- (346) P. R. Bunker, W. P. Kraemer, S. N. Yurchenko, W. Thiel, C. F. Neese, J. L. Gottfried und P. Jensen, *Mol. Phys.* **105**, 1369-1376 (2007).  
New Potential Energy Surfaces for the  $\tilde{X}$  and  $\tilde{A}$  States of CH<sub>2</sub><sup>+</sup>

- (347) Z. Cao, Y. Mo und W. Thiel, *Angew. Chem.* **119**, 6935-6939 (2007); *Angew. Chem., Int. Ed.* **46**, 6811-6815 (2007).  
Deprotonation Mechanism of  $\text{NH}_4^+$  in the *Escherichia coli* Ammonium Transporter AmtB: Insight from QM and QM/MM calculations.
- (348) M. A. Mroginiski, F. Mark, W. Thiel und P. Hildebrandt, *Biophys. J.* **93**, 1885-1894 (2007).  
Quantum Mechanics/Molecular Mechanics Calculation of the Raman Spectra of the Phycocyanobilin Chromophore in  $\alpha$ -C-Phycocyanin.
- (349) S. N. Yurchenko, W. Thiel und P. Jensen, *J. Mol. Spectrosc.* **245**, 126-140 (2007).  
Theoretical ROVibrational Energies (TROVE): A Robust Numerical Approach to the Calculation of Rovibrational Energies for Polyatomic Molecules.
- (350) T. W. Keal, A. Koslowski und W. Thiel, *Theor. Chem. Acc.* **118**, 837-844 (2007).  
Comparison of Algorithms for Conical Intersection Optimisation Using Semiempirical Methods.
- (351) D. P. Geerke, S. Thiel, W. Thiel und W. F. van Gunsteren, *Phys. Chem. Chem. Phys.* **10**, 297-302 (2008).  
QM-MM Interactions in Simulations of Liquid Water using Combined Semi-Empirical/Classical Hamiltonians.
- (352) R. A. Mata, H.-J. Werner, S. Thiel und W. Thiel, *J. Chem. Phys.* **128**, 025104/1-8 (2008).  
Toward Accurate Barriers for Enzymatic Reactions: QM/MM Case Study on *p*-Hydroxybenzoate Hydroxylase.
- (353) S. N. Yurchenko, B. A. Voronin, R. N. Tolchenov, N. Doss, O. V. Naumenko, W. Thiel und J. Tennyson, *J. Chem. Phys.* **128**, 044312/1-12 (2008).  
Potential Energy Surface of HDO up to 25000  $\text{cm}^{-1}$ .
- (354) M. Schreiber, M. R. Silva-Junior, S. P. A. Sauer und W. Thiel, *J. Chem. Phys.* **128**, 134110/1-25 (2008).  
Benchmarks for Electronically Excited States: CASPT2, CC2, CCSD, and CC3.
- (355) T. Tuttle und W. Thiel, *Phys. Chem. Chem. Phys.* **10**, 2159-2166 (2008).  
OMx-D: Semiempirical Methods with Orthogonalization and Dispersion Corrections. Implementation and Biochemical Application.



- (356) D. Wang, J. Zheng, S. Shaik und W. Thiel, *J. Phys. Chem. B* **112**, 5126-5138 (2008).  
Quantum and Molecular Mechanical Study of the First Proton Transfer in the Catalytic Cycle of Cytochrome P450cam and Its Mutant D251N.
- (357) S. N. Yurchenko, W. Thiel, M. Carvajal und P. Jensen, *Chem. Phys.* **346**, 146-159 (2008).  
Ab Initio Potential Energy Surface, Electric Dipole Moment, Polarizability Tensor, and Theoretical Rovibrational Spectra in the Electronic Ground State of  $^{14}\text{NH}_3^+$ .
- (358) M. Mladenovic, K. Junold, R. F. Fink, W. Thiel, T. Schirmeister und B. Engels, *J. Phys. Chem. B* **112**, 5458-5469 (2008).  
Atomistics Insights into the Inhibition of Cysteine Proteases: First QM/MM Calculations Claryfying the Regiospecificity and the Inhibition Potency of Epoxide- and Aziridine-Based Inhibitors.
- (359) E. Fabiano, T. W. Keal und W. Thiel, *Chem. Phys.* **349**, 334-347 (2008).  
Implementation of Surface Hopping Molecular Dynamics using Semiempirical Methods.
- (360) E. Fabiano, G. Groenhof und W. Thiel, *Chem. Phys.* **351**, 111-116 (2008).  
Approximate Switching Algorithms for Trajectory Surface Hopping.
- (361) M. Mladenovic, R. F. Fink, W. Thiel, T. Schirmeister und B. Engels, *J. Am. Chem. Soc.* **130**, 8696-8705 (2008).  
On the Origin of the Stabilization of the Zwitterionic Resting State of Cysteine Proteases: A Theoretical Study.
- (362) E. Fabiano und W. Thiel, *J. Phys. Chem. A* **112**, 6859-6863 (2008).  
Nonradiative Deexcitation Dynamics of 9H-adenine: An OM2 Surface Hopping Study.
- (363) R. I. Ovsyannikov, W. Thiel, S. N. Yurchenko, M. Carvajal und P. Jensen, *J. Chem. Phys.* **129**, 044309/1-8 (2008).  
Vibrational Energies of  $\text{PH}_3$  Calculated Variationally at the Complete Basis Set Limit.
- (364) M. R. Silva-Junior, M. Schreiber, S. P. A. Sauer und W. Thiel, *J. Chem. Phys.* **129**, 104103/1-14 (2008).  
Benchmarks for Electronically Excited States: TD-DFT and DFT/MRCI.

- (365) M. Mladenovic, K. Ansorg, R. F. Fink, W. Thiel, T. Schirmeister und B. Engels, *J. Phys. Chem. B* **112**, 11798-11808 (2008).  
Atomistics Insights into the Inhibition of Cysteine Proteases: First QM/MM Calculations Clarifying the Stereoselectivity of Epoxide-Based Inhibitors.
- (366) T. Benighaus und W. Thiel, *J. Chem. Theory Comput.* **4**, 1600-1609 (2008).  
Efficiency and Accuracy of the Generalized Solvent Boundary Potential for Hybrid QM/MM Simulations: Implementation for Semiempirical Hamiltonians.
- (367) R. I. Ovsyannikov, V. V. Melnikov, W. Thiel, P. Jensen, O. Baum, T. F. Giesen und S. N. Yurchenko, *J. Chem. Phys.* **129**, 154314/1-9 (2008).  
Theoretical Rotation-Torsion Energies of HSOH.
- (368) R. I. Ovsyannikov, W. Thiel, S. N. Yurchenko, M. Carvajal und P. Jensen, *J. Mol. Spectrosc.* **252**, 121-128 (2008).  
PH<sub>3</sub> Revisited: Theoretical Transition Moments for the Vibrational Transitions below 7000 cm<sup>-1</sup>.
- (369) S. Ye, T. Tuttle, E. Bill, L. Simkhovich, Z. Gross, W. Thiel und F. Neese, *Chem. Eur. J.* **14**, 10839-10851 (2008).  
The Electronic Structure of Iron Corroles: A Combined Experimental and Quantum Chemical Study.
- (370) A. Altun, D. Kumar, F. Neese und W. Thiel, *J. Phys. Chem. A* **112**, 12904-12910 (2008).  
Multi-reference Ab Initio QM/MM Study on Intermediates in the Catalytic Cycle of Cytochrome P450<sub>cam</sub>.
- (371) K.-B. Cho, H. Hirao, H. Chen, M. A. Carvajal, S. Cohen, E. Derat, W. Thiel und S. Shaik, *J. Phys. Chem. A* **112**, 13128-13138 (2008).  
Compound I in Heme Thiolate Enzymes: A Comparative QM/MM Study.
- (372) N. Otte, M. Bocola und W. Thiel, *J. Comput. Chem.* **30**, 154-162 (2009).  
Force Field Parameters for the Simulation of Tetrahedral Intermediates of Serine Hydrolases.
- (373) H. M. Senn und W. Thiel, *Angew. Chem.* **121**, 1220-1254 (2009); *Angew. Chem., Int. Ed.* **48**, 1198-1229 (2009).  
QM/MM Methods for Biomolecular Systems.

- (374) W. Thiel, in: *Multiscale Simulation Methods in Molecular Sciences*, J. Grotendorst (Hrsg.), NIC Series, Bd. 42, Jülich, 2009, S. 203-214.  
QM/MM Methodology: Fundamentals, Scope, and Limitations.
- (375) D. Wang und W. Thiel, *J. Mol. Struct.: THEOCHEM* **898**, 90-96 (2009).  
The Oxyheme Complexes of P450cam: A QM/MM Study.
- (376) M. C. Daza, M. Doerr, S. Salzmann, C. M. Marian und W. Thiel, *Phys. Chem. Chem. Phys.* **11**, 1688-1696 (2009).  
Photophysics of Phenalenone: Quantum-mechanical Investigation of Singlet-Triplet Intersystem Crossing.
- (377) Z. Lan, E. Fabiano und W. Thiel, *J. Phys. Chem. B* **113**, 3548-3555 (2009).  
Photoinduced Nonadiabatic Dynamics of Pyrimidine Nucleobases: On-the-fly Surface-Hopping Study with Semiempirical Methods.
- (378) S. P. A. Sauer, M. Schreiber, M. R. Silva-Junior und W. Thiel, *J. Chem. Theory Comput.* **5**, 555-564 (2009).  
Benchmarks for Electronically Excited States: A Comparison of Noniterative and Iterative Triples Corrections – CCSDR(3) versus CC3.
- (379) K. R. Geethalakshmi, M. P. Waller, W. Thiel und M. Bühl, *J. Phys. B* **113**, 4456-4465 (2009).  
<sup>51</sup>V NMR Chemical Shifts Calculated from QM/MM models of Peroxo-forms of Vanadium Haloperoxidases.
- (380) S. Metz, D. Wang und W. Thiel, *J. Am. Chem. Soc.* **131**, 4628-4640 (2009).  
Reductive Half-reaction of Aldehyde Oxidoreductase toward Acetaldehyde: A Combined QM/MM Study.
- (381) M. Altarsha, T. Benighaus, D. Kumar und W. Thiel, *J. Am. Chem. Soc.* **131**, 4755-4763 (2009).  
How is the Reactivity of Cytochrome P450cam Affected by Thr252X Mutation? A QM/MM Study for X = Serine, Valine, Alanine, Glycine.
- (382) T. W. Keal, M. Wanko und W. Thiel, *Theor. Chem. Acc.* **123**, 145-156 (2009).  
Assessment of Semiempirical Methods for the Photoisomerisation of a Protonated Schiff Base.

- (383) Z. Lan, E. Fabiano und W. Thiel, *ChemPhysChem* **10**, 1225-1229 (2009).  
Photoinduced Nonadiabatic Dynamics of 9H-Guanine.
- (384) M. Altarsha, D. Wang, T. Benighaus, D. Kumar und W. Thiel, *J. Phys. Chem. B* **113**, 9577-9588 (2009).  
QM/MM Study of the Second Proton Transfer in the Catalytic Cycle of the D251N Mutant of Cytochrome P450cam.
- (385) M. Alcarazo, C. W. Lehmann, A. Anoop, W. Thiel und A. Fürstner, *Nature Chem.* **1**, 295-301 (2009).  
Coordination Chemistry at Carbon.
- (386) S. N. Yurchenko, R. I. Ovsyannikov, W. Thiel und P. Jensen, *J. Mol. Spectrosc.* **256**, 119-127 (2009).  
Rotation-Vibration Energy Cluster Formation in XH<sub>2</sub>D and XHD<sub>2</sub> Molecules ( X = Bi, P, and Sb).
- (387) T. Tuttle, D. Wang, W. Thiel, J. Köhler, M. Hofmann und J. Weis, *Dalton Trans.* 5894-5901 (2009).  
Ruthenium Based Catalysts for Olefin Hydrosilylation: Dichloro(*p*-cymene)ruthenium and Related Complexes.
- (388) S. Marawske, D. Dörr, D. Schmitz, A. Koslowski, Y. Lu, H. Ritter, W. Thiel, C. A. M. Seidel und R. Kühnemuth, *ChemPhysChem* **10**, 2041-2048 (2009).  
Fluorophores as Optical Sensors for Local Forces.
- (389) S. N. Yurchenko, A. Yachmenev, W. Thiel, O. Baum, T. F. Giesen, V. V. Melnikov und P. Jensen, *J. Mol. Spectrosc.* **257**, 57-65 (2009).  
An *Ab Initio* Calculation of the Vibrational Energies and Transition Moments of HSOH.
- (390) S. Flügge, A. Anoop, R. Goddard, W. Thiel und A. Fürstner, *Chem. Eur. J.* **15**, 8558-8565 (2009).  
Synthesis, Structure and Bonding in Neutral and Cationic 14-Electron Gold-Alkyne  $\pi$ -Complexes.

- (391) H. M. Senn, J. Kästner, J. Breidung und W. Thiel, *Can. J. Chem.* **87**, 1322-1337 (2009).  
Finite-Temperature Effects in Enzymatic Reactions: Insights from QM/MM Free-Energy Simulations.
- (392) W. Thiel, *J. Phys. Chem. A* **113**, 11457-11464 (2009).  
Autobiography.
- (393) S. N. Yurchenko, R. J. Barber, A. Yachmenev, W. Thiel, P. Jensen und J. Tennyson, *J. Phys. Chem. A* **113**, 11845-11855 (2009).  
A Variationally Computed  $T=300$  K Line List for  $\text{NH}_3$ .
- (394) J. Kästner, J. M. Carr, T. W. Keal, W. Thiel, A. Wander und P. Sherwood, *J. Phys. Chem. A* **113**, 11856-11865 (2009).  
DL-FIND: An Open-Source Geometry Optimizer for Atomistic Simulations.
- (395) S. Metz und W. Thiel, *J. Am. Chem. Soc.* **131**, 14885-14902 (2009).  
A Combined QM/MM Study on the Reductive Half-reaction of Xanthine Oxidase: Substrate Orientation and Mechanism.
- (396) T. Benighaus und W. Thiel, *J. Chem. Theory Comput.* **5**, 3114-3128 (2009).  
A General Boundary Potential for Hybrid QM/MM Simulations of Solvated Biomolecular Systems.
- (397) S. Salzmann, M. R. Silva-Junior, W. Thiel und C. Marian, *J. Phys. Chem. B* **113**, 15610-15618 (2009).  
Influence of the LOV Domain on Low-Lying Excited States of Flavin: A Combined Quantum-Mechanics / Molecular-Mechanics Investigation.
- (398) E. Sanchez-Garcia, M. Doerr, Y.-W. Hsiao und W. Thiel, *J. Phys. Chem. B* **113**, 16622-16631 (2009).  
QM/MM Study of the Monomeric Red Fluorescent Protein DsRed.M1.
- (399) M. Parac, M. Doerr, C. M. Marian und W. Thiel, *J. Comput. Chem.* **31**, 90-106 (2010).  
QM/MM Calculation of Solvent Effects on Absorption Spectra of Guanine.

- (400) J. M. Dieterich, H.-J. Werner, R. A. Mata, S. Metz und W. Thiel, *J. Chem. Phys.* **132**, 035101/1-10 (2010).  
Reductive Half-Reaction of Aldehyde Oxidoreductase toward Acetaldehyde: Ab Initio and Free Energy QM/MM Calculations.
- (401) S. Metz und W. Thiel, *J. Phys. Chem. B* **114**, 1506-1517 (2010).  
QM/MM Studies of Xanthine Oxidase: Variations of Cofactor, Substrate, and Active-Site Glu802.
- (402) S. Shaik, S. Cohen, Y. Wang, H. Chen, D. Kumar und W. Thiel, *Chem. Rev.* **110**, 949-1017 (2010).  
P450 Enzymes: Their Structure, Reactivity and Selectivity, Modeled by QM/MM Calculations.
- (403) Q. Sun, M. Doerr, Z. Li, S. C. Smith und W. Thiel, *Phys. Chem. Chem. Phys.* **12**, 2450-2458 (2010).  
QM/MM Studies of the Structural and Energetic Properties of the Far-red Fluorescent Protein HcRed.
- (404) M. Altarsha, T. Benighaus, D. Kumar und W. Thiel, *J. Biol. Inorg. Chem.* **15**, 361-372 (2010).  
Coupling and Uncoupling Mechanisms in the Methoxy-Threonine Mutant of Cytochrome P450cam: A QM/MM Study.
- (405) A. Yachmenev, S. N. Yurchenko, I. Paidarova, P. Jensen, W. Thiel und S. P. A. Sauer, *J. Chem. Phys.* **132**, 114305/1-15 (2010).  
Thermal Averaging of the Indirect Nuclear Spin-Spin Coupling Constants of Ammonia: The Importance of the Large Amplitude Inversion Mode.
- (406) M. Alcarazo, T. Stork, A. Anoop, W. Thiel und A. Fürstner, *Angew. Chem.* **122**, 2596-2600 (2010); *Angew. Chem., Int. Ed.* **49**, 2542-2546 (2010).  
Steering the Surprisingly Modular  $\pi$ -Acceptor Properties of N-Heterocyclic Carbenes: Implications for Gold Catalysis.
- (407) M. R. Silva-Junior, S. P. A. Sauer, M. Schreiber und W. Thiel, *Mol. Phys.* **108**, 453-465 (2010).  
Basis Set Effects on Coupled Cluster Benchmarks of Electronically Excited States: CC3, CCSDR(3) and CC2.

- (408) E. Sanchez-Garcia, M. Doerr und W. Thiel, *J. Comput. Chem.* **31**, 1603-1612 (2010).  
QM/MM Study of the Absorption Spectra of DsRed.M Chromophores.
- (409) H. Bruns, M. Patil, J. Carreras, A. Vázquez, W. Thiel, R. Goddard und M. Alcarazo, *Angew. Chem.* **122**, 3762-3766 (2010); *Angew. Chem., Int. Ed.* **49**, 3680-3683 (2010).  
Synthesis and Coordination Properties of Nitrogen (I)-Based Ligands.
- (410) M. R. Silva-Junior und W. Thiel, *J. Chem. Theory Comput.* **6**, 1546-1564 (2010).  
Benchmark of Electronically Excited States for Semiempirical Methods: MNDO, AM1, PM3, OM1, OM2, OM3, INDO/S and INDO/S2.
- (411) A. Yachmenev, S. N. Yurchenko, P. Jensen, O. Baum, T. F. Giesen und W. Thiel, *Phys. Chem. Chem. Phys.* **12**, 8387-8397 (2010).  
Theoretical Rotation-Torsion Spectra of HSOH.
- (412) S. N. Yurchenko, M. Carvajal, A. Yachmenev, W. Thiel und P. Jensen, *J. Quant. Spectrosc. Radiat. Transfer* **111**, 2279-2290 (2010).  
A Theoretical-Spectroscopy, Ab-Initio-Based Study of the Electronic Ground State of  $^{121}\text{SBH}_3$ .
- (413) M. K. Kesharwani, W. Thiel und B. Ganguly, *J. Phys. Chem. A* **114**, 10684-10693 (2010).  
Probing the Influence of Anomeric Effects on the Lithium Affinity in 1,3-Diaza Systems: A Computational Study.
- (414) A. Anoop, W. Thiel und F. Neese, *J. Chem. Theory Comput.* **6**, 3137-3144 (2010).  
A Local Pair Natural Orbital Coupled Cluster Study of Rh Catalyzed Asymmetric Olefin Hydrogenation.
- (415) M. R. Silva-Junior, M. Schreiber, S. P. A. Sauer und W. Thiel, *J. Chem. Phys.* **133**, 174318/1-13 (2010).  
Benchmarks of Electronically Excited States: Basis Set Effects on CASPT2 Results.
- (416) Y.-W. Hsiao, E. Sanchez-Garcia, M. Doerr und W. Thiel, *J. Phys. Chem. B* **114**, 15413-15423 (2010).  
Quantum Refinement of Protein Structures: Implementation and Application to the Red Fluorescent Protein DsRed.M1.
- (417) D. Kumar, A. Altun, S. Shaik und W. Thiel, *Faraday Discuss.* **148**, 373-383 (2011).  
Water as Biocatalyst in Cytochrome P450.

- (418) T. Benighaus und W. Thiel, *J. Chem. Theory Comput.* **7**, 238-249 (2011).  
Long-Range Electrostatic Effects in QM/MM Studies of Enzymatic Reactions:  
Application of the Solvated Macromolecule Boundary Potential.
- (419) Y.-W. Hsiao und W. Thiel, *J. Phys. Chem. B* **115**, 2097-2106 (2011).  
pB<sub>2</sub> Intermediate of the Photoactive Yellow Protein: Structure and Excitation  
Energies.
- (420) D. Kumar, W. Thiel und S. P. de Visser, *J. Am. Chem. Soc.* **133**, 3869-3882 (2011).  
Theoretical Study on the Mechanism of the Oxygen Activation Process in Cysteine  
Dioxygenase Enzymes.
- (421) S. Metz und W. Thiel, *Coord. Chem. Rev.* **255**, 1085-1103 (2011).  
Theoretical Studies on the Reactivity of Molybdenum Enzymes.
- (422) O. Weingart, Z. Lan, A. Koslowski und W. Thiel, *J. Phys. Chem. Lett.* **2**, 1506-1509  
(2011).  
Chiral Pathways and Periodic Decay in *cis*-Azobenzene Photodynamics.
- (423) A. Yachmenev, S. N. Yurchenko, P. Jensen und W. Thiel, *J. Chem. Phys.* **134**,  
244307/1-11 (2011).  
A New "Spectroscopic" Potential Energy Surface for Formaldehyde in its Ground  
Electronic State.
- (424) Z. Lan, Y. Lu, E. Fabiano und W. Thiel, *ChemPhysChem* **12**, 1989-1998 (2011).  
QM/MM Nonadiabatic Decay Dynamics of 9H-Adenine in Aqueous Solution.
- (425) A. Metzelthin, E. Sánchez-García, Ö. Birer, G. Schwaab, W. Thiel, W. Sander und M.  
Havenith, *ChemPhysChem* **12**, 2009-2017 (2011).  
Acetylene•••Furan Trimer Formation at 0.37 K as a Model for Ultracold Aggregation  
of Non- and Weakly Polar Molecules.
- (426) A. Kazaryan, Z. Lan, L. V. Schäfer, W. Thiel und M. Filatov, *J. Chem. Theory  
Comput.* **7**, 2189-2199 (2011).  
Surface Hopping Excited-State Dynamics Study of the Photoisomerization of a Light-  
Driven Fluorene Molecular Rotary Motor.



- (427) Y. Lu, Z. Lan und W. Thiel, *Angew. Chem.* **123**, 6996-6999 (2011); *Angew. Chem., Int. Ed.* **50**, 6864-6867 (2011).  
Hydrogen Bonding Regulates the Monomeric Nonradiative Decay of Adenine in DNA Strands.
- (428) A. Yachmenev, S. N. Yurchenko, T. Ribeyre und W. Thiel, *J. Chem. Phys.* **135**, 074302/1-13 (2011).  
High-Level *Ab Initio* Potential Energy Surfaces and Vibrational Energies of H<sub>2</sub>CS.
- (429) J. Breidung und W. Thiel, in: *Handbook of High-Resolution Spectroscopies*, Bd. 1, M. Quack und F. Merkt (Hrsg.), Wiley, Chichester, UK, 2011, S. 389-404.  
Prediction of Vibrational Spectra from *Ab Initio* Theory.
- (430) E. Fabiano, Z. Lan, Y. Lu und W. Thiel, in: *Conical Intersections: Theory, Computation and Experiment*, W. Domcke, D. R. Yarkony und H. Köppel (Hrsg.), World Scientific Publishing, Singapore, 2011; Kapitel 12, S. 463-496.  
Nonadiabatic Trajectory Calculations with *Ab Initio* and Semiempirical Methods.
- (431) S. N. Yurchenko, R. J. Barber, J. Tennyson, W. Thiel und P. Jensen, *J. Mol. Spectrosc.* **268**, 123-129 (2011).  
Towards Efficient Refinement of Molecular Potential Energy Surfaces: Ammonia as a Case Study.
- (432) B. Inés, M. Patil, J. Carreras, R. Goddard, W. Thiel und M. Alcarazo, *Angew. Chem.* **123**, 8550-8553 (2011); *Angew. Chem., Int. Ed.* **50**, 8400-8403 (2011).  
Synthesis, Structure, and Reactivity of a Dihydrido Boremium Cation.
- (433) M. Korth und W. Thiel, *J. Chem. Theory Comput.* **7**, 2929-2936 (2011).  
Benchmarking Semiempirical Methods for Thermochemistry, Kinetics, and Non-covalent Interactions: OMx Methods are almost as Accurate and Robust as DFT-GGA Methods for Organic Molecules.
- (434) P. Meletis, M. Patil, W. Thiel, W. Frank und M. Braun, *Chem. Eur. J.* **17**, 11243-11249 (2011).  
Enantioselective and Diastereoselective Tsuji-Trost Allylic Alkylation of Lactones: An Experimental and Computational Study.

- (435) W. Thiel, *Angew. Chem.* **123**, 9382-9384 (2011); *Angew. Chem., Int. Ed.* **50**, 9216-9217 (2011).  
Theoretical Chemistry – Quo Vadis?
- (436) D. Doron, D. T. Major, A. Kohen, W. Thiel und X. Wu, *J. Chem. Theory Comput.* **7**, 3420-3437 (2011).  
Hybrid Quantum and Classical Simulations of the Dihydrofolate Reductase Catalyzed Hydride Transfer Reaction on an Accurate Semi-Empirical Potential Energy Surface.
- (437) T. C. Ramalho, D. H. Pereira und W. Thiel, *J. Phys. Chem. A* **115**, 13504-13512 (2011).  
Thermal and Solvent Effects on NMR Indirect Spin-Spin Coupling Constants of a Prototypical Chagas Disease Drug.
- (438) J. Petůskova, M. Patil, S. Holle, C. W. Lehmann, W. Thiel und M. Alcarazo, *J. Am. Chem. Soc.* **133**, 20758-20760 (2011).  
Synthesis, Structure, and Reactivity of Carbene-Stabilized Phosphorus(III)-Centered Trications  $[L_3P]^{3+}$ .
- (439) J. Cao, R. Bjornsson, M. Bühl, W. Thiel und T. van Mourik, *Chem. Eur. J.* **18**, 184-195 (2012).  
Modelling Zwitterions in Solution: 3-Fluoro- $\gamma$ -Aminobutyric Acid (3F-GABA).
- (440) G. Cui, Z. Lan und W. Thiel, *J. Am. Chem. Soc.* **134**, 1662-1672 (2012).  
Intramolecular Hydrogen Bonding Plays a Crucial Role in the Photophysics and Photochemistry of the GFP Chromophore.
- (441) E. W. Hernández-Rodríguez, E. Sánchez-García, R. Crespo-Otero, A. L. Montero-Alejo, L. A. Montero und W. Thiel, *J. Phys. Chem. B* **116**, 1060-1076 (2012).  
Understanding Rhodopsin Mutations Linked to the *Retinitis Pigmentosa* Disease: a QM/MM and DFT/MRCI Study.
- (442) K. Meier, W. Thiel und W. F. van Gunsteren, *J. Comput. Chem.* **33**, 363-378 (2012).  
On the Effect of a Variation of the Force Field, Spatial Boundary Condition and Size of the QM Region in QM/MM MD Simulations.
- (443) I. Polyak, M. T. Reetz und W. Thiel, *J. Am. Chem. Soc.* **134**, 2732-2741 (2012).  
QM/MM Study on the Mechanism of the Enzymatic Baeyer-Villiger Reaction.

- (444) Z. Lan, Y. Lu, O. Weingart und W. Thiel, *J. Phys. Chem. A* **116**, 1510-1518 (2012).  
Nonadiabatic Decay Dynamics of a Benzylidene Malononitrile.
- (445) H. Gómez, I. Polyak, W. Thiel, J. M. Lluch und L. Masgrau, *J. Am. Chem. Soc.* **134**, 4743-4752 (2012).  
Retaining Glycosyltransferase Mechanism Studied by QM/MM Methods:  
Lipopolysaccharyl- $\alpha$ -1,4-galactosyltransferase C Transfers  $\alpha$ -Galactose via an  
Oxocarbenium Ion-Like Transition State.
- (446) Y. Lu, Z. Lan und W. Thiel, *J. Comput. Chem.* **33**, 1225-1235 (2012).  
Monomeric Adenine Decay Dynamics Influenced by the DNA Environment.
- (447) G. Cui, Y. Lu und W. Thiel, *Chem. Phys. Lett.* **537**, 21-26 (2012).  
Electronic Excitation Energies, Three-State Intersections, and Photodissociation  
Mechanisms of Benzaldehyde and Acetophenone.
- (448) B. Heggen, Z. Lan und W. Thiel, *Phys. Chem. Chem. Phys.* **14**, 8137-8146 (2012).  
Nonadiabatic Decay Dynamics of 9*H*-Guanine in Aqueous Solution.
- (449) X. Wu, A. Koslowski und W. Thiel, *J. Chem. Theory Comput.* **8**, 2272-2281 (2012).  
Semiempirical Quantum Chemical Calculations Accelerated on a Hybrid Multi-core  
CPU-GPU Computing Platform.
- (450) J. A. Gámez, O. Weingart, A. Koslowski und W. Thiel, *J. Chem. Theory Comput.* **8**, 2352-2358 (2012).  
Cooperating Dinitrogen and Phenyl Rotations in *trans*-Azobenzene  
Photoisomerization.
- (451) M. Barbatti, Z. Lan, R. Crespo-Otero, J. J. Szymczak, H. Lischka und W. Thiel, *J. Chem. Phys.* **137**, 22A503/1-14 (2012).  
Critical Appraisal of Excited-State Nonadiabatic Dynamics Simulations of 9*H*-  
Adenine.
- (452) Y.-W. Hsiao, J. Götze und W. Thiel, *J. Phys. Chem. B* **116**, 8064-8073 (2012).  
The Central Role of Gln63 for the Hydrogen Bonding Network and UV-Visible  
Spectrum of the AppA BLUF Domain.

- (453) M. Patil und W. Thiel, *Chem. Eur. J.* **18**, 10408-10418 (2012).  
Origin of Selectivity of Tsuji-Trost Allylic Alkylation of Lactones: Highly Ordered Transition States with Lithium-Containing Enolates.
- (454) R.-Z. Liao und W. Thiel, *J. Phys. Chem. B.* **116**, 9396-9408 (2012).  
Why is the Oxidation State of Iron Crucial for the Activity of Heme-dependent Aldoxime Dehydratase? A QM/MM Study.
- (455) Q. Sun, Z. Li, Z. Lan, C. Pfisterer, M. Doerr, S. Fischer, S. C. Smith und W. Thiel, *Phys. Chem. Chem. Phys.* **14**, 11413-11424 (2012).  
Isomerization Mechanism of the HcRed Fluorescent Protein Chromophore.
- (456) J. B. Schönborn, A. Koslowski, W. Thiel und B. Hartke, *Phys. Chem. Chem. Phys.* **14**, 12193-12201 (2012).  
Photochemical Dynamics of E-iPr-Furylfulgide.
- (457) G. Cui und W. Thiel, *Phys. Chem. Chem. Phys.* **14**, 12378-12384 (2012).  
Nonadiabatic Dynamics of a Truncated Indigo Model.
- (458) H. Teller, M. Corbet, L. Mantilli, G. Gopakumar, R. Goddard, W. Thiel und A. Fürstner, *J. Am. Chem. Soc.* **134**, 15331-15342 (2012).  
One-point Binding Ligands for Asymmetric Gold Catalysis: Phosphoramidites with a TADDOL-Related But Acyclic Backbone.
- (459) R.-Z. Liao und W. Thiel, *J. Chem. Theory Comput.* **8**, 3793-3803 (2012).  
Comparison of QM-Only and QM/MM Models for the Mechanism of Tungsten-dependent Acetylene Hydratase.
- (460) J. Carreras, M. Patil, W. Thiel und M. Alcarazo, *J. Am. Chem. Soc.* **134**, 16753-16758 (2012).  
Exploiting the  $\pi$ -Acceptor Properties of Carbene-Stabilized Phosphorus Centered Trications  $[L_3P]^{3+}$ : Applications in Pt(II) Catalysis.
- (461) T. Saito und W. Thiel, *J. Phys. Chem. A* **116**, 10864-10869 (2012).  
Analytical Gradients for Density Functional Calculations with Approximate Spin Projection.

- (462) E. Boulanger und W. Thiel, *J. Chem. Theory Comput.* **8**, 4527-4538 (2012).  
Solvent Boundary Potentials for Hybrid QM/MM Computations Using Classical Drude Oscillators: A Fully Polarizable Model.
- (463) S. N. Yurchenko, W. Thiel, and Per Jensen, *AIP Conf. Proc.* **1504**, 491-494 (2012).  
Rotation-Vibration Energy Level Cluster Formation in Three- and Four-atomic Molecules.
- (464) G. Cui und W. Thiel, *Angew. Chem.* **125**, 451-454 (2013); *Angew. Chem., Int. Ed.* **52**, 433-436 (2013).  
Photoinduced Ultrafast Wolff Rearrangement: A Non-Adiabatic Dynamics Perspective.
- (465) K. Sen, R. Crespo-Otero, O. Weingart, W. Thiel und M. Barbatti, *J. Chem. Theory Comput.* **9**, 533-542 (2013).  
Interfacial States in Donor-Acceptor Organic Heterojunctions: Computational Insights into Thiophene-Oligomer/Fullerene Junctions.
- (466) C. Grebner, J. Kästner, W. Thiel und B. Engels, *J. Chem. Theory Comput.* **9**, 814-821 (2013).  
A New Tabu-Search-Based Algorithm for Solvation of Proteins.
- (467) R.-Z. Liao und W. Thiel, *J. Phys. Chem. B* **117**, 1326-1336 (2013).  
Determinants of Regioselectivity and Chemoselectivity in Fosfomycin Resistance Protein FosA from QM/MM Calculations.
- (468) I. Čorić, J. H. Kim, T. Vlaar, M. Patil, W. Thiel und B. List, *Angew. Chem.* **125**, 3574-3577 (2013); *Angew. Chem., Int. Ed.* **52**, 3490-3493 (2013).  
Brønsted Acid Catalyzed Asymmetric S<sub>N</sub>2-Type O-Alkylations.
- (469) R. Crespo-Otero, K. Bravo-Rodriguez, S. Roy, T. Benighaus, W. Thiel, W. Sander und E. Sánchez-García, *ChemPhysChem*, **14**, 805-811 (2013).  
Interactions of Aromatic Radicals with Water.
- (470) Á. Kozma, G. Gopakumar, C. Farès, W. Thiel und M. Alcarazo, *Chem. Eur. J.* **19**, 3542-3546 (2013).  
Synthesis and Structure of Carbene-stabilized N-centered Cations [L<sub>2</sub>N]<sup>+</sup>, [L<sub>2</sub>NR]<sup>2+</sup>, [LNR<sub>3</sub>]<sup>2+</sup> and [L<sub>3</sub>N]<sup>3+</sup>.

- (471) J. P. Götze und W. Thiel, *Chem. Phys.* **415**, 247-255 (2013).  
TD-DFT and DFT/MRCI Study of Electronic Excitations in Violaxanthin and Zeaxanthin.
- (472) M. Patil, C. Loerbroks und W. Thiel, *Org. Lett.* **15**, 1682-1685 (2013).  
Mechanism of the Pummerer Reaction: A Computational Study.
- (473) R.-Z. Liao und W. Thiel, *J. Phys. Chem. B* **117**, 3954-3961 (2013).  
On the Effect of Varying Constraints in the QM-Only Modeling of Enzymatic Reactions: the Case of Acetylene Hydratase.
- (474) O. Lifchits, M. Mahlau, C. M. Reisinger, A. Lee, C. Farès, I. Polyak, G. Gopakumar, W. Thiel und B. List, *J. Am. Chem. Soc.* **135**, 6677-6693 (2013).  
The Chinchona Primary Amine-Catalyzed Asymmetric Epoxidation and Hydroperoxidation of  $\alpha,\beta$ -Unsaturated Carbonyl Compounds with Hydrogen Peroxide.
- (475) I. Polyak, M. T. Reetz und W. Thiel, *J. Phys. Chem. B* **117**, 4993-5001 (2013).  
Quantum Mechanical/Molecular Mechanical Study on the Enantioselectivity of the Enzymatic Baeyer-Villiger Reaction of 4-Hydroxycyclohexanone.
- (476) S. Khan, G. Gopakumar, W. Thiel und M. Alcarazo, *Angew. Chem.* **125**, 5755-5758 (2013); *Angew. Chem., Int. Ed.* **52**, 5644-5647 (2013).  
Stabilization of Two-Coordinate  $[\text{GeCl}]^+$  Cation by Simultaneous  $\sigma$  and  $\pi$  Donation from a Monodentate Carbodiphosphorane.
- (477) X. Huang, M. Patil, C. Farès, W. Thiel und N. Maulide, *J. Am. Chem. Soc.* **135**, 7312-7323 (2013).  
Sulfur (IV)-Mediated Transformations: From Ylide Transfer to Metal-Free Arylation of Carbonyl Compounds.
- (478) D. Kumari, H. Singh, M. Patil, W. Thiel, C. S. Pant und S. Banerjee, *Thermochim. Acta* **562**, 96-104 (2013).  
Synthesis, Characterization, Thermal and Computational Studies of Novel Tetra-Azido Esters as Energetic Plasticizers.
- (479) R. C. Fortenberry, X. Huang, A. Yachmenev, W. Thiel und T. J. Lee, *Chem. Phys. Lett.* **574**, 1-12 (2013).  
On the Use of Quartic Force Fields in Variational Calculations.

- (480) D. Audisio, G. Gopakumar, L.-G. Xie, L. G. Alves, C. Wirtz, A. M. Martins, W. Thiel, C. Farès und N. Maulide, *Angew. Chem.* **125**, 6434-6438 (2013); *Angew. Chem., Int. Ed.* **52**, 6313-6316 (2013).  
Palladium-Catalyzed Allylic Substitution at Four Membered Cyclic Systems: Formation of  $\eta^1$ -Allyl Complexes and Electrocyclic Ring Opening.
- (481) L. Spörkel, G. Cui und W. Thiel, *J. Phys. Chem. A* **117**, 4574-4583 (2013).  
Photodynamics of Schiff Base Salicylideneaniline: Trajectory Surface-Hopping Simulations.
- (482) X. Wu, W. Thiel, S. Pezeshki und H. Lin, *J. Chem. Theory Comput.* **9**, 2672-2686 (2013).  
Specific Reaction Path Hamiltonian for Proton Transfer in Water: Reparameterized Semiempirical Models.
- (483) J. A. Gámez, O. Weingart, A. Koslowski und W. Thiel, *Phys. Chem. Chem. Phys.* **15**, 11814-11821 (2013).  
Periodic Decay in the Photoisomerisation of *p*-Aminoazobenzene.
- (484) E. Boulanger, A. Anoop, D. Nachtigallova, W. Thiel und M. Barbatti, *Angew. Chem.* **125**, 8158-8161 (2013); *Angew. Chem., Int. Ed.* **52**, 8000-8003 (2013).  
Photochemical Steps in the Prebiotic Synthesis of Purine Precursors from HCN.
- (485) I. Polyak, E. Boulanger, K. Sen und W. Thiel, *Phys. Chem. Chem. Phys.* **15**, 14188-14195 (2013).  
A Microiterative Intrinsic Reaction Coordinate Method for Large QM/MM Systems.
- (486) I. Polyak, T. Benighaus, E. Boulanger und W. Thiel, *J. Chem. Phys.* **139**, 064104/1-11 (2013).  
Quantum Mechanics/Molecular Mechanics Dual Hamiltonian Free Energy Perturbation.
- (487) R. Marquardt, K. Sagui, J. Zheng, W. Thiel, D. Luckhaus, S. Yurchenko, F. Mariotti und M. Quack, *J. Phys. Chem. A* **117**, 7502-7522 (2013).  
Global Analytical Potential Energy Surface for the Electronic Ground State of NH<sub>3</sub> from High Level ab Initio Calculations.

- (488) M. R. Silva-Junior, M. Mansurova, W. Gärtner und W. Thiel, *ChemBioChem* **14**, 1648-1661 (2013).  
Photophysics of Structurally Modified Flavin Derivates in the Blue-Light Photoreceptor Ytva: A Combined Experimental and Theoretical Study.
- (489) B. Karasulu, M. Patil und W. Thiel, *J. Am. Chem. Soc.* **135**, 13400-13413 (2013).  
Amine Oxidation Mediated by Lysine-Specific Demethylase 1: Quantum Mechanics/Molecular Mechanics Insights into Mechanism and Role of Lysine 661.
- (490) G. Cui, X.-Y. Cao, W.-H. Fang, M. Dolg und W. Thiel, *Angew. Chem.* **125**, 10471-10475 (2013); *Angew. Chem., Int. Ed.* **52**, 10281-10285 (2013).  
Photoinduced Gold(I)–Gold(I) Chemical Bonding in Dicyanoaurate Oligomers.
- (491) R.-Z. Liao und W. Thiel, *J. Comput. Chem.* **34**, 2389-2397 (2013).  
Convergence in the QM-only and QM/MM Modeling of Enzymatic Reactions: A Case Study for Acetylene Hydratase.
- (492) S. N. Yurchenko, J. Tennyson, R. J. Barber und W. Thiel, *J. Mol. Spectrosc.* **291**, 69-76 (2013).  
Vibrational Transition Moments of CH<sub>4</sub> from First Principles.
- (493) D. Escudero, E. Heuser, R. J. Meier, M. Schäferling, W. Thiel und E. Holder, *Chem. Eur. J.* **19**, 15639-15644 (2013).  
Unveiling Photodeactivation Pathways for a New Iridium(III) Cyclometalated Complex.
- (494) C. Loerbroks, R. Rinaldi und W. Thiel, *Chem. Eur. J.* **19**, 16282-16294 (2013).  
The Electronic Nature of 1,4- $\beta$ -Glycosidic Bond and its Chemical Environment: DFT Insights into Cellulose Chemistry.
- (495) W. Thiel, *Nachr. Chem.* **61**, 1095-1096 (2013).  
Komplexe chemische Systeme realistisch modellieren.
- (496) W. Thiel und G. Hummer, *Nature* **504**, 96-97 (2013).  
Nobel 2013 Chemistry: Methods for Computational Chemistry.
- (497) A. Yachmenev, I. Polyak und W. Thiel, *J. Chem. Phys.* **139**, 204308/1-14 (2013).  
Theoretical Rotation-Vibration Spectrum of Thioformaldehyde.



- (498) J. P. Götze, B. Karasulu und W. Thiel, *J. Chem. Phys.* **139**, 234108/1-8 (2013).  
Computing UV/vis Spectra from the Adiabatic and Vertical Franck-Condon Schemes with the Use of Cartesian and Internal Coordinates.
- (499) J. Carreras, G. Gopakumar, A. Gimeno, P. Linowski, J. Petušková, W. Thiel und M. Alcarazo, *J. Am. Chem. Soc.* **135**, 18815-18823 (2013).  
Polycationic Ligands in Gold Catalysis: Synthesis and Applications of Extremely  $\pi$ -Acidic Catalysts.
- (500) W. Thiel, *WIREs Comput. Mol. Sci.* **4**, 145-157 (2014).  
Semiempirical Quantum-Chemical Methods.
- (501) J. A. Gámez, A. Kosłowski und W. Thiel, *RSC Adv.* **4**, 1886-1889 (2014).  
Enhanced E  $\rightarrow$  Z Photoisomerisation in 2-Aminoazobenzene.
- (502) G. Seidel, B. Gabor, R. Goddard, B. Heggen, W. Thiel und A. Fürstner, *Angew. Chem.* **126**, 898-901 (2014); *Angew. Chem., Int. Ed.* **53**, 879-882 (2014) .  
Gold Carbenoids: Lessons Learnt from a Transmetalation Approach.
- (503) L. Spörkel, G. Cui, A. Kosłowski und W. Thiel, *J. Phys. Chem. A* **118**, 152-157 (2014).  
Nonequilibrium H/D Isotope Effects from Trajectory-based Nonadiabatic Dynamics.
- (504) C. M. Marian, S. Nakagawa, V. Rai-Constapel, B. Karasulu und W. Thiel, *J. Phys. Chem. B* **118**, 1743-1753 (2014).  
Photophysics of Flavin Derivatives Absorbing in the Blue-Green Region: Thioflavins as Potential Cofactors of Photoswitches.
- (505) K. Sen und W. Thiel, *J. Phys. Chem. B* **118**, 2810-2820 (2014).  
Role of Two Alternate Water Networks in Compound I Formation in P450eryF.
- (506) E. Boulanger und W. Thiel, *J. Chem. Theory Comput.* **10**, 1795-1809 (2014).  
Toward QM/MM Simulation of Enzymatic Reactions with the Drude Oscillator Polarizable Force Field.
- (507) T. Saito und W. Thiel, *J. Phys. Chem. B* **118**, 5034-5043 (2014).  
Quantum Mechanics/Molecular Mechanics Study of Oxygen Binding in Hemocyanin.

- (508) D. Escudero und W. Thiel, *J. Chem. Phys.* **140**, 194105/1-8 (2014).  
Assessing the density functional theory-based multireference configuration interaction (DFT/MRCI) method for transition metal complexes.
- (509) S. Shaik, H. Chen, D. Usharani und W. Thiel, in: *Drug Metabolism Prediction*, J. Kirchmair (Hrsg.), Wiley-VCH, Weinheim, 2014; Kapitel 6, S. 133-177.  
QM/MM Studies of Structure and Reactivity of Cytochrome P450 Enzymes: Methodology and Selected Applications.
- (510) K. Sen, R. Crespo-Otero, W. Thiel und M. Barbatti, *Comput. Theor. Chem.* **1040-1041**, 237-242 (2014).  
Electronic Structure of Fullerene-Squaraine Complexes for Photovoltaic Devices.
- (511) L. Gu, G. Gopakumar, P. Gualco, W. Thiel und M. Alcarazo, *Chem. Eur. J.* **20**, 8575-8578 (2014).  
Bis- and Tris(pyrazolyl)borate/Methane-Stabilized P<sup>III</sup>-Centered Cations.
- (512) G. Cui und W. Thiel, *J. Phys. Chem. Lett.* **5**, 2682-2687 (2014).  
Intersystem Crossing Enables 4-Thiothymidine to Act as a Photosensitizer in Photodynamic Therapy: An Ab Initio QM/MM Study.
- (513) W. Thiel, *Angew. Chem.* **126**, 8748-8757 (2014); *Angew. Chem., Int. Ed.* **53**, 8605-8613 (2014).  
Computational Catalysis – Past, Present, and Future.
- (514) Q. Zhang, X. Chen, G. Cui, W.-H. Fang und W. Thiel, *Angew. Chem.* **126**, 8793-8797 (2014); *Angew. Chem., Int. Ed.* **53**, 8649-8653 (2014).  
Concerted Asynchronous Hula-Twist Photoisomerization in the S65T/H148D Mutant of Green Fluorescent Protein.
- (515) C. Loerbroks, B. Böker, J. Cordes, A. G. M. Barrett und W. Thiel, *Eur. J. Org. Chem.* 5476-5486 (2014).  
Spiroaminals – Crystal Structure and Computational Investigation of Conformational Preferences and Tautomerization Reactions.
- (516) A. Altun, J. Breidung, F. Neese und W. Thiel. *J. Chem. Theory Comput.* **10**, 3807-3820 (2014).  
Correlated Ab Initio and Density Functional Studies on H<sub>2</sub> Activation by FeO<sup>+</sup>.

- (517) C. Loerbroks, J. van Rijn, M.-P. Ruby, Q. Tong, F. Schüth und W. Thiel, *Chem. Eur. J.* **20**, 12298-12309 (2014).  
Reactivity of Metal Catalysts in Glucose–Fructose Conversion.
- (518) G. Cui und W. Thiel, *J. Chem. Phys.* **141**, 124101/1-13 (2014).  
Generalized Trajectory Surface-Hopping Method for Internal Conversion and Intersystem Crossing.
- (519) A. Nikiforov, J. A. Gamez, W. Thiel, M. Huix-Rotllant und M. Filatov, *J. Chem. Phys.* **141**, 124122/1-16 (2014).  
Assessment of approximate computational methods for conical intersections and branching plane vectors in organic molecules.
- (520) D. Escudero und W. Thiel, *Inorg. Chem.* **53**, 11015-11019 (2014).  
Exploring the Triplet Excited State Potential Energy Surfaces of a Cyclometalated Pt(II) Complex: Is There Non-Kasha Emissive Behavior?
- (521) J. P. Götze, D. Kröner, S. Banerjee, B. Karasulu und W. Thiel, *ChemPhysChem* **15**, 3392-3401 (2014).  
Carotenoids as a Shortcut for Chlorophyll Soret-to-Q Band Energy Flow.
- (522) A. Luzio, D. Fazzi, F. Nübling, R. Matsidik, A. Straub, H. Komber, E. Giussani, S. E. Watkins, M. Barbatti, W. Thiel, E. Gann, L. Thomsen, C. R. McNeill, M. Caironi und M. Sommer, *Chem. Mater.* **26**, 6233-6240 (2014).  
Structure–Function Relationships of High-Electron Mobility Naphthalene Diimide Copolymers Prepared Via Direct Arylation.
- (523) B. Karasulu, J. P. Götze und W. Thiel, *J. Chem. Theory Comput.* **10**, 5549-5566 (2014).  
Assessment of Franck-Condon Methods for Computing Vibrationally Broadened UV-vis Absorption Spectra of Flavin Derivatives: Riboflavin, Roseoflavin, and 5-Thioflavin.
- (524) L. M. Wolf und W. Thiel, *J. Org. Chem.* **79**, 12136-12147 (2014).  
Origin of Inversion versus Retention in the Oxidative Addition of 3-Chlorocyclopentene to Pd(0)L<sub>n</sub>.

- (525) Y. Lu, Z. Lan und W. Thiel, in: Photoinduced Phenomena in Nucleic Acids, M. Barbatti, A. C. Borin und S. Ullrich (Hrsg.), Topics in Current Chemistry, Bd. 356, Springer, Berlin, 2015, S. 89-122.  
Computational Modelling of Photoexcitation in DNA Single and Double Strands.
- (526) B. Karasulu und W. Thiel, J. Phys. Chem. B **119**, 928-943 (2015).  
Photoinduced Intra-molecular Charge Transfer in an Electronically Modified Flavin Derivative: Roseoflavin.
- (527) S. Holle, D. Escudero, B. Inés, J. Rust, W. Thiel und M. Alcarazo, Chem. Eur. J. **21**, 2744-2749 (2015).  
On the Reactivity of Tetrakis(trifluoromethyl)cyclopentadienone towards Carbon-Based Lewis Bases.
- (528) B. Karasulu und W. Thiel, ACS Catal. **5**, 1227-1239 (2015).  
Amine Oxidation Mediated by N-Methyltryptophan Oxidase: Computational Insights into the Mechanism, Role of Active-Site Residues, and Covalent Flavin Binding.
- (529) L. Spörkel, J. Jankowska und W. Thiel, J. Phys. Chem. B **119**, 2702-2710 (2015).  
Photoswitching of Salicylidene Methylamine: A Theoretical Photodynamics Study.
- (530) D. Fazzi, M. Barbatti und W. Thiel, Phys. Chem. Chem. Phys. **17**, 7787-7799 (2015).  
Modeling Ultrafast Exciton Deactivation in Oligothiophenes *via* Nonadiabatic Dynamics.
- (531) C. Loerbroks, E. Boulanger und W. Thiel, Chem. Eur. J. **21**, 5477-5487 (2015).  
Solvent Influence on Cellulose 1,4- $\beta$ -Glycosidic Bond Cleavage: A Molecular Dynamics and Metadynamics Study.
- (532) X.-P. Chang, G. Cui, W.-H. Fang und W. Thiel, ChemPhysChem **16**, 933-937 (2015).  
Mechanism for the Nonadiabatic Photooxidation of Benzene to Phenol: Orientation-Dependent Proton-Coupled Electron Transfer.
- (533) S.-H. Xia, B.-B. Xie, Q. Fang, G. Cui und W. Thiel, Phys. Chem. Chem. Phys. **17**, 9687-9697 (2015).  
Excited-State Intramolecular Proton Transfer to Carbon Atoms: Nonadiabatic Surface-Hopping Dynamics Simulations.

- (534) P. Sokkar, E. Boulanger, W. Thiel und E. Sánchez-García, *J. Chem. Theory Comput.* **11**, 1809-1818 (2015).  
Hybrid Quantum Mechanics/Molecular Mechanics/Coarse Grained Modeling: A Triple-Resolution Approach for Biomolecular Systems.
- (535) C. Loerbroks, A. Heimermann und W. Thiel, *J. Comput. Chem.* **36**, 1114-1123 (2015).  
Solvent Effects on the Mechanism of Cellulose Hydrolysis: a QM/MM Study.
- (536) P. Dral, O. A. von Lilienfeld und W. Thiel, *J. Chem. Theory Comput.* **11**, 2120-2125 (2015).  
Machine Learning of Parameters for Accurate Semiempirical Quantum Chemical Calculations.
- (537) M. G. Schwab, M. Takase, A. Mavrinsky, W. Pisula, X. Feng, J. A. Gámez, W. Thiel, K. S. Mali, S. de Feyter und K. Müllen, *Chem. Eur. J.* **21**, 8426-8434 (2015).  
Torands Revisited: Metal Sequestration and Self-Assembly of Cyclo-2,9-tris-1,10-phenantrolin Hexaaza Macrocycles.
- (538) A. Owens, S. N. Yurchenko, A. Yachmenev, J. Tennyson und W. Thiel, *J. Chem. Phys.* **142**, 244306/1-10 (2015).  
Accurate *Ab Initio* Vibrational Energies of Methyl Chloride.
- (539) A. Owens, S. Yurchenko, W. Thiel und V. Spirko, *Mon. Not. R. Astron. Soc.* **450**, 3191-3200 (2015).  
Accurate Prediction of the Ammonia Probes of a Variable Proton-to-Electron Mass Ratio.
- (540) J. Willwacher, B. Heggen, C. Wirtz, W. Thiel und A. Fürstner, *Chem. Eur. J.* **21**, 10416-10430 (2015).  
Total Synthesis, Stereochemical Revision, and Biological Reassessment of Mandelalide A: Chemical Mimicry of Intrafamily Relationships.
- (541) S. P. A. Sauer, H. F. Pitzner-Frydendahl, M. Buse, H. J. A. Jensen und W. Thiel, *Mol. Phys.* **113**, 2026-2045 (2015).  
Performance of SOPPA-based Methods in the Calculation of Vertical Excitation Energies and Oscillator Strengths.

- (542) D. Escudero, W. Thiel und B. Champagne, *Phys. Chem. Chem. Phys.* **17**, 18908-18912 (2015).  
Spectroscopic and Second-order Nonlinear Optical Properties of Ruthenium(II) Complexes: A DFT/MRCI and ADC(2) Study.
- (543) T. Vasilevskaya, M. G. Khrenova, A. V. Nemukhin und W. Thiel, *J. Comput. Chem.* **36**, 1621-1630 (2015).  
Mechanism of Proteolysis in Matrix Metalloproteinase-2 Revealed by QM/MM Modeling.
- (544) A. Ceausu-Velcescu, P. Pracna, J. Breidung, W. Thiel und M. Badaoui, *J. Mol. Spectrosc.* **316**, 11-21 (2015).  
The  $\nu_4 = 1$  and  $\nu_4 = 2$  Rovibrational Levels of  $\text{PF}_3$  Revisited: New Solutions for Old Topics.
- (545) M. K. Ilg, L. M. Wolf, L. Mantilli, C. Farès, W. Thiel und A. Fürstner, *Chem. Eur. J.* **21**, 12279-12284 (2015).  
A Striking Case of Enantioinversion in Gold Catalysis and Its Probable Origins.
- (546) L.-G. Xie, V. Bagutski, D. Audisio, L. Wolf, V. Schmidts, K. Hofmann, C. Farès, W. Thiel, C. M. Thiele und N. Maulide, *Chem. Sci.* **6**, 5734-5739 (2015).  
Dynamic Behavior of Monohaptoallylpalladium Species: Internal Coordination as a Driving Force in Allylic Alkylation Chemistry.
- (547) J. P. Götze, B. Karasulu, M. Patil und W. Thiel, *Biochim. Biophys. Acta, Bioenerg.* **1847**, 1509-1517 (2015).  
Vibrational Relaxation as the Driving Force for Wavelength Conversion in the Peridinin-Chlorophyll a-Protein.
- (548) M. Leutsch, L. M. Wolf, P. Gupta, M. Fuchs, W. Thiel, C. Farès und A. Fürstner, *Angew. Chem.* **127**, 12608-12613 (2015); *Angew. Chem. Int. Ed.* **54**, 12431-12436 (2015).  
Formation of Ruthenium Carbenes by *gem*-Hydrogen Transfer to Internal Alkynes: Implications for Alkyne *trans*-Hydrogenation.
- (549) L. Liu, M. Leutsch, Y. Zheng, M. W. Alachraf, W. Thiel und B. List, *J. Am. Chem. Soc.* **137**, 13268-13371 (2015).  
Confined Acid-Catalyzed Asymmetric Carbonyl–Ene Cyclization.

- (550) A. Owens, S. N. Yurchenko, O. L. Polyansky, R. I. Ovsyannikov, W. Thiel und V. Spirko, *Mon. Not. R. Astron. Soc.* **454**, 2292-2298 (2015).  
Accurate Prediction of  $\text{H}_3\text{O}^+$  and  $\text{D}_3\text{O}^+$  Sensitivity Coefficients to Probe a Variable Proton-to-Electron Mass Ratio.
- (551) D. T. Mancini, K. Sen, M. Barbatti, W. Thiel und T. C. Ramalho, *ChemPhysChem* **16**, 3444-3449 (2015).  
Excited-State Proton Transfer Can Tune the Color of Protein Fluorescent Markers.
- (552) F. Buchner, B. Heggen, H.-H. Ritze, W. Thiel und A. Lübcke, *Phys. Chem. Chem. Phys.* **17**, 31978-31987 (2015).  
Excited-state Dynamics of Guanosine in Aqueous Solution Revealed by Time-resolved Photoelectron Spectroscopy: Experiment and Theory.
- (553) A. Owens, S. N. Yurchenko, A. Yachmenev und W. Thiel, *J. Chem. Phys.* **143**, 244317/1-12 (2015).  
A Global Potential Energy Surface and Dipole Moment Surface for Silane.
- (554) M. Huix-Rotllant, A. Nikiforov, W. Thiel und M. Filatov, *Top. Curr. Chem.* **368**, 445-476 (2016).  
Description of Conical Intersections with Density Functional Methods.
- (555) X. Wu, A. Koslowski und W. Thiel, in: *Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics*, R. C. Walker und A. W. Goetz (Hrsg.), John Wiley & Sons, Chichester, 2016; Kapitel 11, S. 239-257.  
Semiempirical Quantum Chemistry.
- (556) B. Heggen, M. Patil und W. Thiel, *J. Comput. Chem.* **37**, 280-285 (2016).  
Cyclization of an  $\alpha,\beta$ -Unsaturated Hydrazone Catalyzed by a BINOL-Phosphoric Acid: Pericyclic or Not?
- (557) A. Nikiforov, J. A. Gamez, W. Thiel und M. Filatov, *J. Phys. Chem. Lett.* **7**, 105-110 (2016).  
Computational Design of a Family of Light-Driven Rotary Molecular Motors with Improved Quantum Efficiency.

- (558) B. Heggen und W. Thiel, *J. Organomet. Chem.* **804**, 42-47 (2016).  
Theoretical Investigation on the Mechanism of Iron Catalyzed Cross Coupling Reactions via Ferrate Intermediates.
- (559) M. Patil und W. Thiel, *Eur. J. Org. Chem.*, 830-839 (2016).  
Mechanism of Ylide Transfer to Carbonyl Compounds: Density Functional Calculations.
- (560) S.-H. Xia, G. Cui, W.-H. Fang und W. Thiel, *Angew. Chem.* **128**, 2107-2112 (2016);  
*Angew. Chem. Int. Ed.* **55**, 2067-2072 (2016).  
How Photoisomerization Drives Peptide Folding and Unfolding: Insights from QM/MM and MM Dynamics Simulations.
- (561) X.-Y. Liu, X.-P. Chang, S.-H. Xia, G. Cui und W. Thiel, *J. Chem. Theory Comput.* **12**, 753-764 (2016).  
Excited-State Proton-Transfer-Induced Trapping Enhances the Fluorescence Emission of Locked GFP Chromophore.
- (562) S. Henkel, P. Costa, L. Klute, P. Sokkar, M. Fernandez-Oliva, W. Thiel, E. Sanchez-Garcia und W. Sander, *J. Am. Chem. Soc.* **138**, 1689-1697 (2016).  
Switching the Spin State of Diphenylcarbene via Halogen Bonding.
- (563) P. O. Dral, X. Wu, L. Spörkel, A. Koslowski, W. Weber, R. Steiger, M. Scholten und W. Thiel, *J. Chem. Theory Comput.* **12**, 1082-1096 (2016).  
Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Theory, Implementation, and Parameters.
- (564) P. O. Dral, X. Wu, L. Spörkel, A. Koslowski und W. Thiel, *J. Chem. Theory Comput.* **12**, 1097-1120 (2016).  
Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Benchmarks for Ground-State Properties.
- (565) D. Fazzi, M. Barbatti und W. Thiel, *J. Am. Chem. Soc.* **138**, 4502-4511 (2016).  
Unveiling the Role of Hot Charge-Transfer States in Molecular Aggregates via Nonadiabatic Dynamics.



- (566) E. Boess, L. M. Wolf, S. Malakar, M. Salamone, M. Bietti, W. Thiel und M. Klusmann, *ACS Catal.* **6**, 3253-3261 (2016).  
Competitive Hydrogen Atom Transfer to Oxyl- and Peroxyl Radicals in the Cu-Catalyzed Oxidative Coupling of *N*-Aryl Tetrahydroisoquinolines Using *tert*-Butyl Hydroperoxide.
- (567) A. Owens, S. N. Yurchenko, W. Thiel und V. Špirko, *Phys. Rev. A* **93**, 052506/1-5 (2016).  
Enhanced Sensitivity to a Possible Variation of the Proton-to-Electron Mass Ratio in Ammonia.
- (568) L. Spörkel und W. Thiel, *J. Chem. Phys.* **144**, 194108/1-8 (2016).  
Adaptive Time Steps in Trajectory Surface Hopping Simulations.
- (569) Y. Guo, F. E. Beyle, B. M. Bold, H. C. Watanabe, A. Koslowski, W. Thiel, P. Hegemann, M. Marazzi und M. Elstner, *Chem. Sci.* **7**, 3879-3891 (2016).  
Active Site Structure and Absorption Spectrum of Channelrhodopsin-2 Wild-Type and C128T Mutant.
- (570) J. W. Dube, Y. Zheng, W. Thiel und M. Alcarazo, *J. Am. Chem. Soc.* **138**, 6869-6877 (2016).  
 $\alpha$ -Cationic Arsines: Synthesis, Structure, Reactivity, and Applications.
- (571) T. Vasilevskaya, M. G. Khrenova, A. V. Nemukhin und W. Thiel, *J. Comput. Chem.* **37**, 1801-1809 (2016).  
Methodological Aspects of QM/MM Calculations: A Case Study on Matrix Metalloproteinase-2.
- (572) L. Kötzner, M. Leutsch, S. Sievers, S. Patil, H. Waldmann, Y. Zheng, W. Thiel und B. List, *Angew. Chem.* **128**, 7824-7828 (2016); *Angew. Chem. Int. Ed.* **55**, 7693-7697 (2016).  
The Organocatalytic Approach to Enantiopure *2H*- and *3H*-Pyrroles: Inhibitors of the Hedgehog Signaling Pathway.
- (573) T. Vasilevskaya, M. G. Khrenova, A. V. Nemukhin und W. Thiel, *Mendeleev Commun.* **26**, 209-211 (2016).  
Reaction Mechanism of Matrix Metalloproteinases with a Catalytically Active Zinc Ion Studied by the QM(DFTB)/MM Simulations.

- (574) S. Das, L. Liu, Y. Zheng, M. W. Alachraf, W. Thiel, C. K. De und B. List, *J. Am. Chem. Soc.* **138**, 9429-9432 (2016).  
Nitrated Confined Acids Enable a Catalytic Asymmetric Oxa-Pictet-Spengler Reaction.
- (575) A. Owens, S. N. Yurchenko, A. Yachmenev, J. Tennyson und W. Thiel, *J. Quant. Spectrosc. Radiat. Transfer* **184**, 100-110 (2016).  
A Global *Ab Initio* Dipole Moment Surface for Methyl Chloride.
- (576) T. Vasilevskaya und W. Thiel, *J. Chem. Theory Comput.* **12**, 3561-3570 (2016).  
Periodic Boundary Conditions in QM/MM Calculations: Implementation and Tests.
- (577) X.-P. Chang, Y.-Y. Zheng, G. Cui, W.-H. Fang und W. Thiel, *Phys. Chem. Chem. Phys.* **18**, 24713-24721 (2016).  
Photocycloaddition Reaction of Atropisomeric Maleimides: Mechanism and Selectivity.
- (578) A. Owens, S. N. Yurchenko, A. Yachmenev, J. Tennyson und W. Thiel, *J. Chem. Phys.* **145**, 104305/1-13 (2016).  
A Highly Accurate *Ab Initio* Potential Energy Surface for Methane.
- (579) A. Ganguly, C. C. Manahan, D. Top, E. F. Yee, C. Lin, M. W. Young, W. Thiel und B. R. Crane, *Proc. Nat. Acad. Sci. USA* **113**, 10073-10078 (2016).  
Changes in Active Site Histidine Hydrogen Bonding Trigger Cryptochrome Activation.
- (580) D. Tuna, Y. Lu, A. Koslowski und W. Thiel, *J. Chem. Theory Comput.* **12**, 4400-4422 (2016).  
Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Benchmarks of Electronically Excited States.
- (581) J. Knorr, P. Sokkar, S. Schott, P. Costa, W. Thiel, W. Sander, E. Sanchez-Garcia und P. Nuernberger, *Nat. Commun.* **7**, 12968 (2016).  
Competitive Solvent-Molecule Interactions Govern Primary Processes of Diphenylcarbene in Solvent Mixtures.

- (582) Y.-T. Wang, X.-Y. Liu, G. Cui, W.-H. Fang und W. Thiel, *Angew. Chem.* **128**, 14215-14219 (2016); *Angew. Chem., Int. Ed.* **55**, 14009-14013 (2016).  
Photoisomerization of Arylazopyrazole Photoswitches: Exclusive Chiral Excited-State Relaxation.
- (583) S. Kahmann, D. Fazzi, G. J. Matt, W. Thiel, M. A. Loi und C. J. Brabec, *J. Phys. Chem. Lett.* **7**, 4438-4444 (2016).  
Polarons in Narrow Band-Gap Polymers Probed over the Entire Infrared Range: A Joint Experimental and Theoretical Investigation.
- (584) F. Lombeck, H. Komber, D. Fazzi, D. Nava, J. Kuhlmann, D. Stegerer, K. Strassel, J. Brandt, J. Lenz, A. Lederer, A. D. de Zerio Mendaza, C. Müller, W. Thiel, M. Caironi, R. Friend und M. Sommer, *Adv. Energy Mat.* **6**, 1601232 / 1-9.  
On the Effect of Prevalent Carbazole Homocoupling Defects on the Photovoltaic Performance of PCDTBT:PC<sub>71</sub>BM Solar Cells.
- (585) Y. Xie, G.-J. Cheng, S. Lee, P. S. J. Kaib, W. Thiel und B. List, *J. Am. Chem. Soc.* **138**, 14538-14541 (2016).  
Catalytic Asymmetric Vinylogous Prins Cyclization: A Highly Diastereo- and Enantioselective Entry to Tetrahydrofurans.
- (586) M. R. Monaco, D. Fazzi, N. Tsuji, M. Leutzsch, S. Liao, W. Thiel und B. List, *J. Am. Chem. Soc.* **138**, 14740-14749 (2016).  
The Activation of Carboxylic Acids via Self-Assembly Asymmetric Organocatalysis: A Combined Experimental and Computational Investigation.
- (587) S. Wang, H. Sun, U. Ail, M. Vagin, P. O. Å. Persson, J. W. Andreasen, W. Thiel, M. Berggren, X. Crispin, D. Fazzi und S. Fabiano, *Adv. Mater.* **28**, 10764-10771 (2016).  
Thermoelectric Properties of Solution-Processed n-Doped Ladder-Type Conducting Polymers.
- (588) G. König, F. C. Pickard, J. Huang, A. C. Simmonett, F. Tofoleanu, J. Lee, P. O. Dral, S. Prasad, M. Jones, Y. Shao, W. Thiel und B. R. Brooks, *J. Comput. Aided Mol. Des.* **30**, 989-1006 (2016).  
Calculating Distribution Coefficients Based on Multi-scale Free Energy Simulations: An Evaluation of MM and QM/MM Explicit Solvent Simulations of Water-Cyclohexane Transfer in the SAMPL5 Challenge.

- (589) A. M. Escorcia, K. Sen, M. C. Daza, M. Doerr und W. Thiel, *ACS Catal.* **7**, 115-127 (2017).  
Quantum Mechanics/Molecular Mechanics Insights into the Enantioselectivity of the *O*-Acetylation of (*R,S*)-Propranolol Catalyzed by *Candida antarctica* Lipase B.
- (590) X. Gao und W. Thiel, *Phys. Rev. E* **95**, 013308 / 1-7 (2017).  
Non-Hermitian Surface Hopping.
- (591) J. F. Hitzenberger, P. O. Dral, U. Meinhardt, T. Clark, W. Thiel, M. Kivala und T. Drewello, *ChemPlusChem* **82**, 204-211 (2017).  
Stability of Odd- Versus Even-Electron Gas-Phase (Quasi)Molecular Ions Derived from Pyridine-Substituted N-Heterotriangulenes.
- (592) X. Gao, S. Bai, D. Fazzi, T. Niehaus, M. Barbatti und W. Thiel, *J. Chem. Theory Comput.* **13**, 515-524 (2017).  
Evaluation of Spin-Orbit Couplings with Linear-Response Time-Dependent Density Functional Methods.
- (593) D.-A. Roşca, K. Radkowski, L. M. Wolf, M. Wagh, R. Goddard, W. Thiel und A. Fürstner, *J. Am. Chem. Soc.* **139**, 2443-2455 (2017).  
Ruthenium-Catalyzed Alkyne *trans*-Hydrometalation: Mechanistic Insights and Preparative Implications.
- (594) A. Ganguly, W. Thiel und B. Crane, *J. Am. Chem. Soc.* **139**, 2972-2980 (2017).  
Glutamine Amide Flip Elicits Long Distance Allosteric Responses in the LOV Protein Vivid.
- (595) S. M. Rummelt, G. Cheng, P. Gupta, W. Thiel und Alois Fürstner, *Angew. Chem.* **129**, 3653-3658 (2017); *Angew. Chem. Int. Ed.* **56**, 3599-3604 (2017).  
Hydroxy-Directed Ruthenium-Catalyzed Alkene/Alkyne Coupling: Increased Scope, Stereochemical Implications, and Mechanistic Rationale.
- (596) L. Gu, L. M. Wolf, A. Zieliński, W. Thiel und M. Alcarazo, *J. Am. Chem. Soc.* **139**, 4948-4953 (2017).  
 $\alpha$ -Dicationic Chelating Phosphines: Synthesis and Application to the Hydroarylation of Dienes.

- (597) Y.-J. Gao, X.-P. Chang, X.-Y. Liu, Q.-S. Li, G. Cui und W. Thiel, *J. Phys. Chem. A* **121**, 2572-2579 (2017).  
Excited-State Decay Paths in Tetraphenylethene Derivatives.
- (598) A. Ganguly, E. Boulanger und W. Thiel, *J. Chem. Theory Comput.* **13**, 2954-2961 (2017).  
Importance of MM Polarization in QM/MM Studies of Enzymatic Reactions: Assessment of the QM/MM Drude Oscillator Model.
- (599) P. O. Dral, A. Owens, S. N. Yurchenko und W. Thiel, *J. Chem. Phys.* **146**, 244108/1-11 (2017).  
Structure-based Sampling and Self-correcting Machine Learning for Accurate Calculations of Potential Energy Surfaces and Vibrational Levels.
- (600) A. Ganguly, T. Q. Luong, O. Brylski, M. Dirkmann, D. Möller, S. Ebbinghaus, F. Schulz, R. Winter, E. Sanchez-Garcia und W. Thiel, *J. Phys. Chem. B* **121**, 6390-6398 (2017).  
Elucidation of the Catalytic Mechanism of a Miniature Zinc Finger Hydrolase.
- (601) L. Gu, Y. Zheng, E. Haldon, R. Goddard, E. Bill, W. Thiel und M. Alcarazo, *Angew. Chem.* **129**, 8916-8920 (2017); *Angew. Chem. Int. Ed.* **56**, 8790-8794 (2017).  
 $\alpha$ -Radical Phosphines: Synthesis, Structure, and Reactivity.
- (602) X.-P. Chang, Y.-J. Gao, W.-H. Fang, G. Cui und W. Thiel, *Angew. Chem.* **129**, 9469-9473 (2017); *Angew. Chem. Int. Ed.* **56**, 9341-9345 (2017).  
Quantum Mechanics/Molecular Mechanics Study on the Photoreactions of Dark- and Light-Adapted States of a Blue-Light YtvA LOV Photoreceptor.
- (603) V. Pattni, T. Vasilevskaya, W. Thiel und M. Heyden, *J. Phys. Chem. B* **121**, 7431-7442 (2017).  
Distinct Protein Hydration Water Species Defined by Spatially Resolved Spectra of Intermolecular Vibrations.
- (604) B. D. Gliemann, V. Strauss, J. F. Hitzenberger, P. O. Dral, F. Hampel, J.-P. Gisselbrecht, T. Drewello, W. Thiel, D. M. Guldi und M. Kivala, *Chem. Eur. J.* **23**, 12353-12363 (2017).  
Dithiafulvenyl-Extended N-Heterotriangulenes and Their Interaction with C<sub>60</sub>: Cooperative Fluorescence.

- (605) A. Owens, A. Yachmenev, W. Thiel, J. Tennyson und S. N. Yurchenko, *Mon. Not. R. Astron. Soc.* **471**, 5025-5032 (2017).  
ExoMol Line Lists – XXII. The Rotation-Vibration Spectrum of Silane up to 1200 K.
- (606) D. Fazzi, M. Barbatti und W. Thiel, *J. Phys. Chem. Lett.* **8**, 4727-4734 (2017).  
Hot and Cold Charge Transfer Mechanisms in Organic Photovoltaics: Insights into the Excited States of Donor/Acceptor Interfaces.
- (607) N. Drosos, G. Cheng, E. Ozkal, B. Cacherat, W. Thiel und B. Morandi, *Angew. Chem.* **129**, 13562-13566 (2017); *Angew. Chem. Int. Ed.* **56**, 13377-13381 (2017).  
Catalytic Reductive Pinacol-Type Rearrangement of Unactivated 1,2-Diols through a Concerted, Stereoinvertive Mechanism.
- (608) E. Decaneto, T. Vasilevskaya, Y. Kutin, H. Ogata, M. Grossman, I. Sagi, M. Havenith, W. Lubitz, W. Thiel und N. Cox, *Phys. Chem. Chem. Phys.* **19**, 30316-30331 (2017).  
Solvent Water Interactions within the Active Site of the Membrane Type I Matrix Metalloproteinase.
- (609) Y. Zheng und W. Thiel, *J. Org. Chem.* **82**, 13563-13571 (2017).  
Computational Insights into an Enzyme-Catalyzed [4+2] Cycloaddition.
- (610) G. Cheng, N. Drosos, B. Morandi und W. Thiel, *ACS Catal.* **8**, 1697-1702 (2018).  
Computational Study of B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>-Catalyzed Selective Deoxygenation of 1,2-Diols: Cyclic and Noncyclic Pathways.
- (611) A. Guthertz, M. Leutzsch, L. M. Wolf, P. Gupta, S. M. Rummelt, R. Goddard, C. Farès, W. Thiel und A. Fürstner, *J. Am. Chem. Soc.* **140**, 3156-3169 (2018).  
Half-Sandwich Ruthenium Carbene Complexes Link *trans*-Hydrogenation and *gem*-Hydrogenation of Internal Alkynes.
- (612) L. Gu, L. M. Wolf, W. Thiel, C. W. Lehmann und M. Alcarazo, *Organometallics* **37**, 665-672 (2018).  
Reductive Elimination of C<sub>6</sub>F<sub>5</sub>-C<sub>6</sub>F<sub>5</sub> from Pd(II) Complexes: Influence of  $\alpha$ -Dicationic Chelating Phosphines.
- (613) D. Wu, Y.-T. Wang, W.-H. Fang, G. Cui und W. Thiel, *Chem. Asian J.* **13**, 780-784 (2018).  
QM/MM Studies on the Photoisomerization Dynamics of Azobenzene Chromophore Tethered to a DNA Duplex: Local Unpaired Nucleobase Plays a Crucial Role.

- (614) J. Liu und W. Thiel, *J. Chem. Phys.* **148**, 154103/1-12 (2018).  
An Efficient Implementation of Semiempirical Quantum-chemical Orthogonalization-corrected Methods for Excited-state Dynamics.
- (615) P. Armengol, L. Spörkel, R. Gelabert, M. Moreno, W. Thiel und J. M. Lluch, *Phys. Chem. Chem. Phys.* **20**, 11067-11080 (2018).  
Ultrafast Action Chemistry in Slow Motion: Atomistic Description of the Excitation and Fluorescence Processes in an Archetypal Fluorescent Protein.
- (616) A. M. Escorcia, J. P. M. van Rijn, G. Cheng, P. Schrepfer, T. B. Brück und W. Thiel, *J. Comput. Chem.* **39**, 1215-1225 (2018).  
Molecular Dynamics Study of Taxadiene Synthase Catalysis.
- (617) J. Liu, A. Koslowski und W. Thiel, *J. Chem. Phys.* **148**, 244108/1-11 (2018).  
Analytic Gradient and Derivative Couplings for the Spin-flip Extended Configuration Interaction Singles Method: Theory, Implementation, and Application to Proton transfer.
- (618) G. König, M. T. Reetz und W. Thiel, *J. Phys. Chem. B* **122**, 6975-6988 (2018).  
1-Butanol as a Solvent for Efficient Extraction of Polar Compounds from Aqueous Medium: Theoretical and Practical Aspects.
- (619) G. König, B. R. Brooks, W. Thiel und D. M. York, *Mol. Simul.* **44**, 1062-1081 (2018).  
On the Convergence of Multi-Scale Free Energy Simulations.
- (620) G. Bistoni, I. Polyak, M. Sparta, W. Thiel und F. Neese, *J. Chem. Theory Comput.* **14**, 3524-3531 (2018).  
Toward Accurate QM/MM Reaction Barriers with Large QM Regions Using Domain Based Pair Natural Orbital Coupled Cluster Theory.
- (621) A. Owens, A. Yachmenev, W. Thiel, A. Fateev, J. Tennyson und S. N. Yurchenko, *Mon. Not. R. Astron. Soc.* **479**, 3002-3010 (2018).  
ExoMol Line Lists – XXIX. The Rotation-Vibration Spectrum of Methyl Chloride up to 1200 K.
- (622) P. O. Dral, M. Barbatti und W. Thiel, *J. Phys. Chem. Lett.* **9**, 5660-5663 (2018).  
Nonadiabatic Excited-State Dynamics with Machine Learning.

- (623) G. König, F. C. Pickard IV, J. Huang, W. Thiel, A. D. MacKerell, Jr., B. R. Brooks und D. M. York, *Molecules* **23**, 2695/1-25 (2018).  
A Comparison of QM/MM Simulations with and without the Drude Oscillator Model Based on Hydration Free Energies of Simple Solutes.
- (624) P. Xiao, C.-X. Li, W.-H. Fang, G. Cui und W. Thiel, *J. Am. Chem. Soc.* **140**, 15099-15113 (2018).  
Mechanism of the Visible-Light-Mediated Copper-Catalyzed Coupling Reaction of Phenols and Alkynes.
- (625) A. Owens, A. Yachmenev, J. Küpper, S. N. Yurchenko und W. Thiel, *Phys. Chem. Chem. Phys.* **21**, 3496-3505 (2019).  
The Rotation-Vibration Spectrum of Methyl Fluoride from First Principles.
- (626) D. Tuna, L. Spörkel, M. Barbatti und W. Thiel, *Chem. Phys.*, online, DOI: 10.1016/j.chemphys.2018.09.036.  
Insights into the Photoisomerization and Excited-State Deactivation Processes of Urocanic Acid: An OM2/MRCI Trajectory-Surface-Hopping Dynamics Study.
- (627) X. Wu, P. O. Dral, A. Kosłowski und W. Thiel, *J. Comput. Chem.* **40**, 638-649 (2019).  
Big Data Analysis of *ab initio* Molecular Integrals in the Neglect of Diatomic Differential Overlap Approximation.
- (628) P. O. Dral, X. Wu und W. Thiel, *J. Chem. Theory Comput.*, 2019, **15** (3), pp 1743–1760  
Semiempirical Quantum-Chemical Methods with Orthogonalization and Dispersion Corrections
- (629) J. Breidung und W. Thiel, *J. Phys. Chem. C* **123**, 7940-7951 (2019).  
Equilibrium Structures of s-Triazine, Pyrazine, and s-Tetrazine.
- (630) Q. Lu, J. Song, P. Wu, C. Li und W. Thiel, *ACS Catal.* **9**, 4892-4901 (2019).  
Mechanistic Insights into the Directing Effect of Thr303 in Ethanol Oxidation by Cytochrome P450 2E1.
- (631) J. P. M. van Rijn, A. M. Escorcia und W. Thiel, *J. Comput. Chem.* **40**, 1902-1910 (2019).  
QM/MM Study of the Taxadiene Synthase Mechanism.



- (632) J. Breidung und W. Thiel, *J. Phys. Chem. A* **123**, 5600-5612 (2019).  
Equilibrium Structures of the Phosphorus Trihalides  $\text{PF}_3$  and  $\text{PCl}_3$ , and the  
Phosphoranes  $\text{PH}_3\text{F}_2$ ,  $\text{PF}_5$ ,  $\text{PCl}_3\text{F}_2$ , and  $\text{PCl}_5$ .