

## Publications: Prof. Dr. Walter Thiel

2018

- (621) A. Owens, A. Yachmenev, W. Thiel, A. Fateev, J. Tennyson, and 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.
- (620) G. Bistoni, I. Polyak, M. Sparta, W. Thiel, and F. Neese, *J. Chem. Theory Comput.* **14**, 3524-3531 (2018).  
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- (619) G. König, B. R. Brooks, W. Thiel; and D. M. York, *Mol. Simul.* **44**, 1062-1081 (2018).  
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1-Butanol as a Solvent for Efficient Extraction of Polar Compounds from Aqueous Medium: Theoretical and Practical Aspects.
- (617) J. Liu, A. Koslowski, and 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.
- (616) A. M. Escorcia, J. P. M. van Rijn, G. Cheng, P. Schrepfer, T. B. Brück, and W. Thiel, *J. Comput. Chem.* **39**, 1215-1225 (2018).  
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- (613) D. Wu, Y.-T. Wang, W.-H. Fang, G. Cui, and 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.
- (612) L. Gu, L. M. Wolf, W. Thiel, C. W. Lehmann, and 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.
- (611) A. Guthertz, M. Leutzsch, L. M. Wolf, P. Gupta, S. M. Rummelt, R. Goddard, C. Farès, W. Thiel, and A. Fürstner, *J. Am. Chem. Soc.* **140**, 3156-3169 (2018).  
Half-Sandwich Ruthenium Carbene Complexes Link *trans*-Hydrogenation and *gem*-Hydrogenation of Internal Alkynes.
- (610) G. Cheng, N. Drosos, B. Morandi, and W. Thiel, *ACS Catal.* **8**, 1697-1702 (2018).  
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- (604) B. D. Gliemann, V. Strauss, J. F. Hitzenberger, P. O. Dral, F. Hampel, J.-P. Gisselbrecht, T. Drewello, W. Thiel, D. M. Guldi, and M. Kivala, *Chem. Eur. J.* **23**, 12353-12363 (2017).  
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