

# Publications by Dominik Marx and by the Marx Lab

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Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum; February 7, 2012

## Contents

<b>1 Peer Reviewed Publications</b>	<b>2</b>
<b>2 Invited Reviews, Features, and Lecture Notes</b>	<b>28</b>
<b>3 Monographs</b>	<b>33</b>
<b>4 Edited Books and Special Issues</b>	<b>33</b>
<b>5 Independent Publications by Members of the Marx Lab</b>	<b>35</b>

## 1 Peer Reviewed Publications

- [•] S. BRAUN, M. BÖCKMANN, AND D. MARX,  
*Unfolding a Photoswitchable Azo-Foldamer Reveals a Non-Covalent Reaction Mechanism*,  
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- [157] M. FARNESI CAMELLONE AND D. MARX,  
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*Quantum Molecular Dynamics Calculations of Ultrafast Timescales and Infrared Spectra of Protonated Methane: Quantifying Isotope-Specific Lifetimes*,  
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*Force-Transformed Free-Energy Surfaces and Trajectory-Shooting Simulations Reveal the Mechano-Stereochemistry of Cyclopropane Ring-Opening Reactions*,  
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- [152] M. FARNESI CAMELLONE, P. M. KOWALSKI, AND D. MARX,  
*Ideal, defective, and gold-promoted rutile TiO<sub>2</sub>(110) surfaces interacting with CO, H<sub>2</sub>, and H<sub>2</sub>O: Structures, energies, thermodynamics, and dynamics from PBE+U*,  
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- [150] R. POLLET, N. N. NAIR, AND D. MARX,  
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- [146] J. KISS, J. FRENZEL, N. N. NAIR, B. MEYER, AND D. MARX,  
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- [143] S. A. FIETHEN, V. STAEMMLER, N. N. NAIR, J. RIBAS-ARINO, E. SCHREINER, AND D. MARX,  
*Revealing the Magnetostructural Dynamics of [2Fe-2S] Ferredoxins from Reduced-Dimensionality Analysis of Antiferromagnetic Exchange Coupling Fluctuations*,  
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- [139] M. HEYDEN, J. SUN, S. FUNKNER, G. MATHIAS, H. FORBERT, M. HAVENITH, AND D. MARX,  
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