UniSysCat - Colloquium

Prof. Dr. Michael Römelt

Humbold-Universität zu Berlin, Institut für Chemie, Theoretische Chemie

Start Time: Wednesday, December 1, 2021 05:00 pm

End Time: Wednesday, December 1, 2021 06:00 pm

Online Colloquium

Quantum Chemistry of Complex Molecular Systems: Relative Spin State Energies and Photoswitches

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Complex molecular systems such as polynuclear transition metal complexes and photochromic compounds play a key role in many areas of chemistry. Yet understanding and predicting their properties as well as their reactivity is a great challenge and one of the current frontiers of theoretical chemistry.[1] The first part of this talk will focus on recent developments in multireference electronic structure theory[2,3] and how it can be used to correctly predict relative spin state energies in transition metal complexes.[4,5] In this context, an example related to Fe-mediated cross coupling reactions will highlight the importance of the total spin state for the reactivity of transition metal compounds. The second part of this talk will be concerned with a recent computational study of the photoinduced isomerization of donor-acceptor Stenhouse adducts (DASAs) that lead to new insight into multiple facets of the reaction mechanism.[6] A central aspect of our work in this regard was to reveal the delicate balance between neutral and zwitterionic resonance structures that governs the relative barrier height for the crucial C2–C3 and C3–C4 bond rotations.

[1] A. Khedkar, M. Roemelt Phys. Chem. Chem. Phys. 2021, 23, 17097-17112

[2] A. Khedkar, M. Roemelt J. Chem. Theory Comput. 2019, 15, 3522-3536

[3] A. Khedkar, M. Roemelt J. Chem. Theory Comput. 2020, 16, 4993-5005

[4] M. Roemelt, V. Krewald, D. A. Pantazis J. Chem. Theory. Comput. 2018, 14, 166-179

[5] A. Khedkar, M. Roemelt Phys. Chem. Chem. Phys. 2020, 22, 17677-17686

[6] M. Ugandi, M. Roemelt, J. Phys. Chem. A 2020, 124, 7756-7767

Prof. Dr. Holger Dobbek

Organizer