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Unifying Concepts in Catalysis

UniCat Colloquium

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The dehydrogenase and hydrogenase activities of Cu/Mo-dependent CO-dehydrogenases: a theoretical perspective

The Mo/Cu-dependent CO dehydrogenase from O. carboxydovorans is an enzyme which is able to catalyze CO oxidation to CO2; moreover, it can also oxidize H2, thus eliciting a characteristic EPR signal. In a recent communication, we used a DFT model of the enzyme active site to characterize H2 coordination to the Cu(I) ion, which was shown not to occur on the same active-ready state competent for CO binding.
In my seminar, I will show recent theoretical results on the activation of H2 on the Mo/Cu binuclear site. Several possible protonation states of key residues in the first and second coordination spheres were considered, which led us to identify heterolytic routes based either on the preliminary side-on coordination of H2 to the metal, or on the presence of a frustrated Lewis pair. The results obtained also inspired us to explore novel possibilities for a better understanding of the CO oxidation catalytic mechanism.

Wednesday, December 13, 2017 at 5:15 PM
TU Berlin, Institute of Chemistry
Straße des 17. Juni 115, 10623 Berlin

Building C, Lecture Hall **C 264**

Prof. Dr. Mroginski (TUB)
Organizer

Coffee and cake will be served 30 minutes before the lecture. Guests are cordially invited to attend!
Prof. Dr. Matthias Driess - Chair of the Cluster of Excellence UniCat - www.unicat.tu-berlin.de