

UniCat Colloquium

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Insights into the oxidative power of lignin-degrading enzymes from QM/MM calculations

Valorization of lignin, a large-scale biowaste in the paper industry, is a major challenge for chemistry. In nature, degradation of this complex polymer is initiated by fungal enzymes. Most of these enzymes that have been characterized to date are heme-based oxidases such as lignin peroxidase (LiP), believed to contain an oxoiron(IV) center in the active compound. After briefly discussing methodological aspects of computing redox potentials for such metal complexes using quantum chemistry [1], we present a QM/MM study of the redox potential of the active compound of LiP [2], believed to be crucial for the biocatalytic activity. Special attention is called to the effects of charged residues around the active site on this property. The calculations can rationalize the observed pH-dependence of the oxidative activity of LiP and can be used to predict possible mutants with increased oxidative power.

[1] L. Castro, M. Bühl, J. Chem. Theor. Comput. 2014, 10, 243-251.

[2] L. Castro, L. Crawford, A. Mutengwa, J. Götze, M. Bühl, Org. Biomol. Chem. 2016, in press (DOI: 10.1039/C6OB00037A)

Wednesday, March 23, 2016 at 5:15 PM

TU Berlin, Institute of Chemistry
Straße des 17. Juni 115, 10623 Berlin

Building C, Lecture Hall **C 264**

Prof. Kaupp (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

