

Donnerstag, 02.06.2022

Hörsaal D, Chemiezentralgebäude, 10:15 Uhr

Sprecher: Ricardo Mata
(*Universität Göttingen*)

Titel: Coupling of proton dynamics to reaction pathways in biomolecular systems

Abstract:

In this talk I will be reviewing some of our most recent works in modelling enzyme catalysis through hybrid quantum chemical approaches. The examples will include two decarboxylase enzymes[1] and the human transketolase.[2] The systems share a common trait. Their function/proficiency builds upon the use of protons to balance local (transient) electrostatic potentials. While for a large body of chemistry a protic medium is an added complication, enzymes have evolved over millennia to embrace protons and skilfully use their lability. By means of QM/MM dynamics and careful evaluation of pKa values in silico, we are able to finally close decades-old discussions on some of these challenging biomolecular riddles. Future perspectives on the use of multicomponent methods and the coupling of the different timescales for these processes will be also discussed.

[1] S. Dai, L.-M. Funk, F. R. von Pappenheim, V. Sautner, M. Paulikat, B. Schröder, J. Uranga, R. A. Mata and K. Tittmann, Low-barrier hydrogen bonds in enzyme cooperativity, *Nature* 573, 609-613 (2019).

[2] S. Rindfleisch, M. Krull, J. Uranga, T. Schmidt, F. Rabe von Pappenheim, L. L. Kirck, A. Balouri, T. Schneider, A. Chari, R. Kluger, G. Bourenkov, U. Diederichsen, R. A. Mata and K. Tittmann, Ground-state destabilization by electrostatic repulsion is not a driving force in orotidine-5'-monophosphate decarboxylase catalysis, *Nat. Catal.* doi: 10.1038/s41929-022-00771-w (2022)

Organisation: B. Engels