Extra Session of Focus Materialchemie – Tuesday, **16.11.2023** 13:00 – @ Seminarraum BA 02B (TU-Wien, Getreidemarkt 9, BC, OG. 02, room A46) – join us on ZOOM (ID: 983 0066 2349)

Electronic Structure Analyses of Iron Complexes for Electrocatalytic Oxygen Reduction

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Catalysts for the efficient activation and transformation of small molecules are essential stepping stones towards a future society that is independent of fossil resources. Fuel cells, for instance for automotive applications, rely on the oxygen reduction reaction. While cost-intensive platinum-based catalysts are considered state-of-the-art, single-atom catalysts (SACs) have shown competitive activity albeit at lower stabilities. SACs are prepared by pyrolysis of earth-abundant precursors and rendered as amorphous powders, which significantly hampers the precise identification of active sites and hence a strategic optimisation of activity and stability.[1]

For Fe-SACs, the active sites are considered as single iron ions ligated by four nitrogen donors embedded in a graphene-like environment. Open questions concern the number and nature of axial ligands and the presence of dopants. This talk will illustrate how quantum chemistry and theoretical spectroscopy can aid in unravelling the identity of active sites. The influence of ligand field strengths on spectroscopic properties will be discussed for complexes with pyridinic and pyrrolic nitrogen donors, including the first iron complex with a pyridinic, conjugated, square-pyramidal coordination sphere.[2-4] The implications for the discernibility of such active sites in *in situ* and *operando* experiments will be discussed.[5-7]

References

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