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New insights on the identification of iron structures in Fe-N-C catalysts by NIS and Mössbauer spectroscopy

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In proton exchange fuel cells (PEFC) the hydrogen oxidation reaction and oxygen reduction reaction are catalysed by platinum-based catalysts. However, for economic reasons it is anticipated to replace platinum on the cathode for the oxygen reduction reaction (ORR). Fe N C catalysts are the most prominent substitute. Molecular FeN4 centres were identified by different groups as ORR active sites [1-5]. However, the oxidation state and structure remains under debate, but it is crucial for further improvement of Fe-N-C catalysts. Recently, we were able to show that sulphite ions can be used as poison for Fe-N-C catalysts [6]. The comparison of different catalysts gives indications of systematic changes in the iron signature. However, due to the ambident character of sulphite ions the interpretation is not straight forward.
In order to get additional insights, temperature dependent Mössbauer spectroscopy and Nuclear Inelastic Scattering (NIS), were used to refine our model of iron sites present in these catalysts. DFT calculations are used to modulate the partial density of iron states (pDOS).
On the basis of this we are able to identify some identic and some changing iron sites in the as-prepared and poisoned catalyst, that gives new insights on the nature of ORR activity in Fe-N-C catalysts.
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