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The role and analysis of molecular systems in electrocatalysis

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Propositions

accompanying the thesis

The role and analysis of molecular systems in electrocatalysis

- 1.** XPS reference spectra of bulk metallic material or metal oxides are not sufficient to unambiguously assign oxidation states to molecular complexes and deposits generated by those (Chapters 2 and 3).
- 2.** The equilibrium redox potential of copper complexes cannot be unequivocally used to predict the overpotential, rate, or selectivity of an electrocatalytic reaction. (Chapters 4 and 5).
- 3.** The geometry of a molecular complex has a larger impact on catalysis than the electron donating or withdrawing effect of the ligand (Chapters 4 and 5).
- 4.** A platinum ring electrode in a rotating ring disk setup is not suitable for determining the Faradaic efficiency of H_2O_2 of long experiments (Chapter 4).
- 5.** A pitfall of purely computational research is that one can easily miss out on events such as catalyst degradation and as a result report a theoretical mechanism that will never take place. (Fonseca, S.; Moreira de Campos Pinto, L. *ACS Omega* 2020, 5, 3, 1581–1585 and Chapter 3).
- 6.** (Electro)catalytic studies of molecular complexes should not be performed at a pH where the ligands are protonated and thereby unable to form a molecular complex in the first place. (Thorseth, M. A.; Letko, C. S.; Tse, E. C. M.; Rauchfuss, T. B.; Gewirth, A. A., *Inorg. Chem.* **2013**, 52, 628–634.)

- 7.** When the only performed characterization of the active species already disagrees with the intended molecular complex, you cannot claim that the catalytic activity stems from that molecular complex. (Thorum, M., Yadav, J. and Gewirth, A. *Angew. Chem. Int. Ed.* **2009**, 48, 165–167 and Chapter 3).
- 8.** Using multiple techniques strengthens conclusions, but can disproportionally increase the time it takes to perform the research.
- 9.** Instead of emphasizing on the contrast between homogeneous and heterogeneous catalysis, these fields of chemistry should focus on the overlap between them.
- 10.** Only a few days of general lab skills training is not enough to become an experimental chemist.
- 11.** At the end of your PhD, new insights will always make you reconsider your previously chosen experimental conditions.
- 12.** One benefit of a pandemic induced lockdown is that you cannot distract yourself from writing your PhD thesis by doing experiments. A downside is that you cannot do experiments to write about in your thesis.

Bas van Dijk