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Title of Lecture: Theory of multi-electron transfer reactions: implications for electrocatalysis

Abstract: Practically all relevant electrocatalytic reactions require the transfer of at least two electrons, and often more than two. A full theory of such reactions does not only require knowledge of the activation energy associated with the event of a single electron, i.e. Marcus theory and its various extensions, but also insight into the relative energies of the intermediate states, i.e. the thermodynamics of all intermediates and the associated elementary steps in which they are formed. Based on this idea, I will show that are fundamental differences in the catalysis of reactions involving 1, 2 or more than 2 electrons, or, partly equivalently, reactions involving 0, 1, or 2 or more catalytic intermediates. For the latter two classes, knowing the thermodynamics of the full reaction is more important than the ability to predict the activation energy of a single step, and in fact the optimal catalyst is first and foremost that material that is able to generate a “thermodynamic landscape” that does not have a sink or mountain. In essence, this is a multidimensional Sabatier principle for the optimal catalyst. The principle will be illustrated on a few examples of important electrocatalytic reactions.