

## Heterogeneous Molecular Catalysis in Electrochemical Reactions Volcanic tafel plots and catalysis tafel plots

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### Abstract

By plotting the kinetics of the catalytic reaction against the stabilisation free energy of the primary intermediate of the catalytic process, we study the reasons for the occurrence or non-occurrence of volcanoes in the context of heterogeneous molecular catalysis. Modern energy challenges, particularly those involving small molecules like water, hydrogen, oxygen, proton, and carbon dioxide, are a strong incentive for such research, as are homogeneous molecular catalysis and catalysis by surface active metallic sites. This is especially true in the case of heterogeneous molecular catalysis, which is typically preferred over homogeneous molecular catalysis by the same molecules, if only for chemical separation and the creation of electrolytic cells.

### Introduction

The volcano plot technique, like the other two catalysis types, relies on the basic premise that kinetic reactions are dependent on a single descriptor, namely the stabilisation free energy of the primary intermediate. More detailed approaches that study reactions under a wide range of experimental circumstances and may be expressed as catalytic Tafel graphs should clearly be preferred. This is especially true in heterogeneous molecular catalysis, where additional transport factors in the supporting film may affect current-potential responses [1]. This is supported by the presence of maxima in catalytic Tafel plots and their reliance on the cyclic voltammetric scan rate. An ever-increasing number of molecular systems, mostly transition metal complexes, are proposed for catalysing electrochemical reactions, particularly the oxidation or reduction of small molecules such as water, hydrogen, oxygen, proton, and carbon dioxide, in the context of today's energy challenges [2]. Although homogeneous molecular catalysis is a promising technology, films containing the same molecules that are applied to the electrode surface are likely to be preferred, if only to facilitate product separation. Another argument is that such catalytic electrodes may be used in complete electrolytic cells, complete with counter electrodes and separators, and can be used with existing electrolyzer and fuel cell technologies. We can anticipate rapid development of this type of device by immobilising molecules that have been demonstrated to be effective homogenous molecular catalysts onto the electrode surface. When it comes to catalyst benchmarking, it has been demonstrated that it can be efficiently operated using catalytic Tafel plots that relate the turnover frequency to the overpotential for each system under consideration [3]. It's unclear how this method, which was developed for homogeneous molecular catalysts, can be applied to deposited molecular catalysts. In terms of the second point, analogies with surface-active site catalysis on the one hand and homogeneous molecule catalysis on the other point to the hypothesis that the

stability of the intermediate created in the initial phase of the reaction may be the most important element in catalytic efficiency. Increasing the intermediate's stability should result in two opposing impacts. One is to lower the energy barrier for the production of the intermediate in a favourable way. The other is that a high level of intermediate stabilisation slows the conversion of the intermediate into products and the subsequent regeneration of the catalytic surface. This "Sabatier principle" predicts the presence of a maximum, or "volcano," on the plot of exchange current vs. adsorption free energy of the intermediate among a family of electrocatalysts for a particular process. These ideas have been around since the late 1950s, yet they are still the subject of intense discussion and controversy today. Their application to homogeneous molecular catalysis is relatively new, and we must take care in the transition to molecular film catalysis. Taking into account the numerous ways of connection between modes of transport Reactants, charges, and catalytic reactions are all discussed. We explore scenarios in which the catalytic reaction is the rate-determining factor at the expense of charge and reactant transport in order to focus on the possible occurrence of volcano plots in the context of molecular film catalysis (the film behaves as a monolayer or as a set of identically behaving monolayers). To get down to the nitty-gritty of the appearance or nonappearance of such volcanic plots, we'll first look at a simple molecular catalysis one-electron-one-step reaction scheme.

## REFERENCES

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