Theoretical Description of Simple Electrode Processes

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Theoretical description of simple electrode processes

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A method is introduced for calculating the stability of reaction intermediates of electrochemical processes as a function of bias on the basis of electronic structure calculations. The method is used in combination with detailed density functional theory (DFT) calculations to develop a description of the free energy landscape of electrochemical electrode processes of relevance to PEM fuel cells. A physical picture is developed of the trends in the electrocatalytic activity of different transition metals for hydrogen oxidation and oxygen reduction.