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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.