Scaling relations in electrocatalysis: from basics to opportunities

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Oxygen reduction remains one of the most intensively studied reactions in electrochemical energy conversion. A main reason is the challenging trade-off in catalyst design due to scaling relations between adsorption energies for reaction intermediates, such as OH and OOH. These relations define a "path" on the ORR activity “volcano”, restricting the optimization of catalytic activity with the chemical space of catalysts.

In this presentation, we will advance from basics through implications to opportunities. We will explore what the scaling relations are, how they emerge from thermodynamic and geometric considerations, and why they constrain catalytic performance. We will employ an original classification of strategies for manipulating the scaling relations to link theory with experiment and distinguish between electronic and geometric effects.

We will oversee how by tuning **inter-site distance, local curvature, and active-site environments** modifies interactions of intermediates with the surface, in special cases, even bypassing the scaling relations. While most of the insights come from the **density functional theory** calculations, insights, we will review a growing number of experimental confirmations.

Through this talk, the audience will:

- Learn what scaling relations are and why they matter.
- Get acquainted with five general strategies for manipulating them.
- See how geometric parameters emerge as a new variable in catalysis.
- Gain insight into how theory and experiment can work together to design catalysts.
- Discover how geometry-driven catalysts can boost ORR.

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