**Recent Developments in ORR Catalysis**

### Introduction
- Oxygen Reduction Reaction (ORR) is a key chemical process fuel cells and metal air batteries.
- Platinum-free catalysts will boost large-scale applications.
- Here: overview of the last developments (2023 and 2024).

**What Is the Rate-Limiting Step of Oxygen Reduction Reaction on Fe–N–C Catalysts?**[1]
- Single iron atoms embedded in nitrogen-doped graphene (Fe–N–C).
- Constant potential AIMD (VASP, so-called "constant-potential hybrid solvation-dynamic model", or CP-HS-DM).
  - Before \( \text{O}_2 \) can adsorb, the Fe-site is already occupied by a water molecule.
  - At TS, \( \text{O}_2 \) and \( \text{H}_2\text{O} \) are bound to Fe.
  - This is a new perspective on the reaction mechanism. \( \text{O}_2 \) (\( \text{H}_2\text{O} \)) adsorption (desorption) occur at once, not in two steps.
  - That step is supposed to be **the rate determining step**!
  - The activation barrier for this step is potential dependent!
  - **But:** no comments on spin states.

### First-Principles Landscape of Single Atomic Catalysts to Metal Catalysts [2]
- PBE-D3 study (zero potential) on intermediate adsorption energies with different catalysts.
- **Formation energies:** DAC1 very stable.
- **Results:** Adsorption energies of reaction intermediates; Scaling relationships + Volcano plots.
  - For some catalysts, a new pathway was proposed.
  - High catalytic activities around SAC/DACS and Pt-NP.

### Enhanced Activity for the Oxygen Reduction Reaction in Microporous Water [3]
- Low solubility of \( \text{O}_2 \) in water limits achievable current densities.
- Idea: introduce a porous solid with *hydrophilic* external surface+ *hydrophobic* internal surface → **aqueous porous liquid** (zeolitic nanocrystals = silicalite-1-NCs).
- \( \text{O}_2 \) is physisorbed on the (large) surface.
- Current densities are increased by a factor of 3.9 with silicate added.
- Reason: The diffusion coefficient of the zeolite is much larger than that of \( \text{O}_2 \) → **better mass transport**. Comparison with different particle size + particle types (hydrophilic internal surface does not work).