MODELING OF BIFUNCTIONAL OXYGEN ELECTROCATALYSIS IN CARBONIZED MOFS

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The development of rechargeable metal-air batteries is necessary for efficient energy storage systems. An essential part is the catalyst material required to efficiently drive oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) occurring during the battery operation. The current challenge is to produce such bifunctional catalyst in a cost-efficient manner without relying on platinum-group metals. One of the proposed alternatives is non-precious metal single-site catalysts obtained from carbonizing metal-organic frameworks (MOFs). Although there exist computational models, essential effects are often neglected. In this study, we compared different methods to account for solvation in density functional theory (DFT) calculations in single-metal catalysts. The proper inclusion of solvent effects allowed us to describe thermodynamic limitations of bifunctional activity more accurately. We compared the obtained ORR and OER activities for different metal centres (Fe, Ni, Co) and considered the energetics of the undesirable H_2O_2 side reaction.

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