Molecular Modelling of Cage Catalysts for CO_2 Reduction

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The increasing atmospheric CO_2 levels correlated with global warming have stimulated efforts to develop technologies cutting its global emissions by decreasing its production or by capturing it. CO_2 can then be used as feedstock. Electrochemical reduction is one of the most promising approaches for CO_2 processing. However, improvements of the efficiency and selectivity of related catalysts are needed.

This presentation focuses on metalloporphyrins and their cages. Their catalytic performance can be tuned by complexation with cations present in electrolyte solutions. By means of ab initio calculations, ab initio and classical molecular dynamics (MD) simulations, we study selected catalysts and reaction intermediates in different electrolytes. The presentation focuses on classical MD and subsequent trajectory analysis. Simulations reveal how exactly different cations interact with the catalysts and also show their rich conformational space. Obtained results provide molecular level insight into functioning of such environmentally relevant catalysts.