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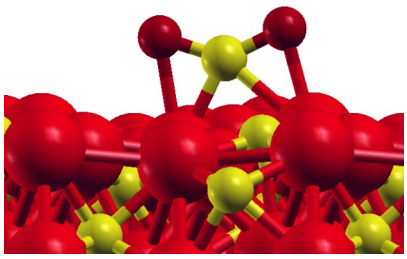
Mechanistic insights into the effect of cobalt doping in iron carbide catalysts for the direct conversion of carbon dioxide to valuable products

Aim

The aim of the study is to identify how the selectivity of iron carbide catalysts change as a function of cobalt loading and the resulting modifications in surface properties, adsorbate coverages and key elementary reactions based on Density Functional Theory (DFT) calculations.

Justification

Iron based catalysts offer a combination of good selectivity and moderate activity in direct conversion of CO_2 to different products. Introduction of cobalt to the iron carbide phase can result in increased activity and the tuning of the product spectrum towards different products. Nevertheless, the complex structures of the bimetallic iron-cobalt carbide surfaces hinder a molecular view of the surface processes, which are crucially needed for a rational optimization of the catalytic performance[1]. The challenge lies in in the identification of different surface structures that are formed as a result of Co-doping to the iron carbide phase and understanding how these structures affect the elementary reactions. Due to the dynamic nature of the active catalytic surface and their complexity, the structure-activity relationships have to be determined by molecular modeling (DFT calculations)[2], guided by experimental characterization. These relationships will guide the rational design of bimetallic catalysts with optimal selectivity to desired products.



Structure of adsorbed CO_2 on a representative iron carbide surface from preliminary DFT results

Program

- Conduct a literature review on iron-cobalt bimetallic catalysts in CO_2 conversion.
- Perform DFT calculations to identify surface structures formed on iron carbides as a function of Co-doping.
- Identify the key performance descriptors of surfaces such as band structures, adsorbate interactions and reaction kinetic parameters.
- Translate the findings to structure-activity relationships between iron-cobalt carbide catalyst formulations and different desired products.

References
1) K.T. Rommens and M. Saeys, Chem. Rev., 2023, 2023, 123, 9, 5798–5858.
2) D. Tuncer and A.C. Kizilkaya, Catalysts 2023, 13, 1390.

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