Potential and challenges of ab initio simulations in CO_2 electroreduction

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CO_2 reduction has become a vital area of research due to its potential to mitigate global warming, with electrocatalytic conversion to chemicals being a key focus. Nonetheless, designing effective electrocatalysts with high selectivity remains a challenge. Advancements in computing capabilities now enable intensive ab initio simulations at the atomic scale, providing valuable insights into electrocatalytic systems. This abstract presents recent findings on the capabilities and challenges of ab initio simulations in understanding the thermodynamics and kinetics of these systems.

The combination of Density Functional Theory calculations with atomistic thermodynamics has allowed to gain insights into the active surfaces of tin-based electrocatalysts under operational conditions, shedding light on factors influencing their performance.
Going beyond the thermodynamic approach, the employment of transition state theory and solvation models permits to estimate the kinetics of CO_2 reduction on metallic electrodes, aiding in the interpretation of experimental results.

These approaches represent a step further in the modelling of complex electrochemical systems and allow for a better understanding of complex phenomena, though still presenting important challenges that must be addressed in the future.