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CO2 hydrogenation on Ru-functionalized Zeolites: Development of Reactive Force Fields and Molecular Dynamics Simulations

We present the development of a new ReaxFF reactive force field parametrization tailored for modelling CO_2 hydrogenation on ruthenium-functionalized zeolites. The force field is based on the CHOAlSi ReaxFF parameters and was reparametrized using extensive DFT data from a prior study, which characterized key elementary steps leading to CO, CH_4, CH_3OH, CH_2O and HCOOH gas products on a single Ru atom embedded in silicalite (Ru_1@S-1). Parameter optimization was carried out using the ParAMS module within the Amsterdam Modeling Suite, targeting accurate reproduction of DFT-calculated reaction energies, geometries and transition states [1]. The resulting force field was validated against the DFT dataset and employed in reactive molecular dynamics simulations to investigate product distributions under controlled temperature, pressure and CO_2/H_2 partial pressures. Additionally, the influence of increasing Ru loading on catalytic performance was explored. This work provides a transferable and computationally efficient tool for studying complex reaction networks in Ru-zeolite catalysts

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