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ReaxFF development for rWGS reaction on Ni/Cu alloys: Effects of Cu content and distribution

The reverse Water-Gas Shift (rWGS) reaction enables the conversion of CO2 into CO, a key intermediate for e-fuel synthesis. Ni-based catalysts are active for rWGS but suffer from limited selectivity due to the competing methanation reaction. In contrast, Cu-based catalysts exhibit high selectivity but lower activity. Alloying these metals has been explored as a strategy to improve the catalyst performance. To gain deeper insight into the behaviour of these types of catalysts, we developed ReaxFF reactive force field parameters. The new Ni/Cu/C/O/H_2025 force field was built on our previously developed force field for rWGS on Ni, alongside parameters from a previously published force field for Cu catalysts. To re-optimize the parameters, we used DFT calculations as reference data alongside optimization algorithms such as the GA-ANN hybrid method (Genetic Algorithm - Artificial Neural Network). Our simulations examined how surface composition and atomic distribution influence catalyst performance. On a (100) surface, a Cu:Ni ratio of 1:3 resulted in catalytic behaviour comparable to pure Ni(100), while increasing Cu content to 1:1 reduced activity by ˜30% but significantly enhanced selectivity, decreasing side product formation by nearly 50%. Dynamic simulations at various temperatures enabled the construction of Arrhenius plots, yielding apparent activation energies in close agreement with DFT values. Additionally, we analysed hydrogen distribution across different surface structures, finding that NiCu alloys exhibit higher subsurface H concentrations than pure Ni, potentially impacting H_2 adsorption and desorption. Finally, we analysed different reaction pathways for CO2 activation and CO desorption that are related with the origin of the selectivity towards CO formation.

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