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Search for molecular corks beyond carbon monoxide: A quantum mechanical study of N-Heterocyclic carbene adsorption on single atom alloys (SAAs)

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Abstract

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Abstract

Periodic Density Functional Theory calculations reveal the potential application of 10 imidazole based N-heterocyclic carbenes (NHCs) to behave as “molecular corks” for hydrogen storage on single atom alloys, comprised of Pd/Cu(111) or Pt/Cu(111). Calculations show that functionalizing the NHC with different electron withdrawing/donating functional groups results in different binding energies of the NHC with the alloy surfaces. The results are compared to DFT calculations of carbon monoxide bound to these alloys. The Huynh electronic parameter (HEP) is calculated for several simple imidazole NHCs to gauge σ-donor ability, while Se-NMR and P-NMR calculations of selenourea derivatives and carbene-phosphinidene adducts, respectively, have been utilized to gauge π-acidity of the NHCs. It is demonstrated that consideration of both σ and π donating/accepting ability must be considered when predicting the surface-adsorbate binding energy. It was found that electron withdrawing groups tend to weaken the NHC-surface interaction while electron donating substituents tend to strengthen the interaction.

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