

[← All Submissions](#)

SUBMISSION

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

[Scott Simpson](#) 0 views 0 downloads

Video

PDF



Abstract



0 Datasets

PRESENTED AT

ACS Spring 2022

Mar 20-24, 2022

EXPLORE MORE CONTENT FROM

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.

Discussion

Ask a Question

Get involved to find out more about this Presentation.

All Comments ▼

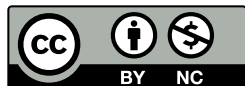
Create an Account or Log In to participate in the discussion

Sign Up

Log In

[Home](#) [Sessions](#) [Submissions](#) [People](#) [Exhibitors](#)

License



Attribution-NonCommercial 4.0 International (CC BY-NC 4.0)

Powered by **Morressier**

Discover more research and events on [morressier.com](https://www.morressier.com)