



Showcasing research from Professors Tonner-Zech, Heine, and Asmis, members of the Research Training Group on Hydrogen Isotopes centred at Leipzig University, Saxony, Germany.

Direct evidence for ligand-enhanced activity of Cu(I) sites

In a combined experimental and computational effort, we study the strength and isotopologue selectivity of hydrogen adsorption on the undercoordinated copper (I) site. Exploiting gas-phase complexes as model systems, we show that the high isotopologue selectivity in dihydrogen binding results from a large difference in the adsorption zero-point energies. We discuss the role of the environment and the coordination geometry of the adsorption site in achieving a high selectivity and the ramifications for identifying and designing future materials for adsorptive dihydrogen isotopologue separation.

As featured in:



See Jiaye Jin, Ralf Tonner-Zech, Thomas Heine, Knut R. Asmis *et al.*, *Chem. Sci.*, 2024, 15, 14635.