Enantiospecific Chemistry of Aspartic acid on Copper Surfaces

Soham Dutta¹ and Andrew J. Gellman^{*,1,2} ¹Department of Chemical Engineering, ²W.E. Scott Institute for Energy Innovation, Carnegie Mellon University, Pittsburgh, PA 15213, USA *** Corresponding Author:** gellman@cmu.edu

Supplementary information

1. In figure 1, temperature programmed reaction spectra (TPRS) of aspartic acid (Asp) enantiomers, namely D-Asp and isotopically labelled L-Asp on Cu(643)^{R&S} are shown.¹ There is a statistically significant difference in the peak temperatures as indicated by the 95% confidence interval values, revealing enantiospecific decomposition kinetics. Each spectra is an average of six spectra and the bands represent one standard deviation at each temperature.



Figure 1

2. The enantiomeric excess of the gas phase (ee_g) in equilibrium with enantiomeric excess on the surface (ee_s) , determined from equilibrium adsorption experiments is plotted in figure 2 for Asp on Cu(111) (green diamonds), Cu(653)^{R&S} (black circles) and Cu(3,1,17)^{R&S} (solid red triangles). On Cu(3,1,17)^{R&S}, there is no aggregation of Asp enantiomers since the surface enantiospecifically adsorbs either L- or D-Asp depending on whether it is Cu(3,1,17)^R or Cu(3,1,17)^S. For Cu(111) and Cu(653)^{R&S}, while ee_s (0) = 0, $ee_s \neq ee_g$ otherwise thus indicating enantiomer aggregation. This isotherm has been modelled using a cluster-adsorption model to determine



Figure 2

References

- 1. Chemical Communication, 2016, 52, 14125
- 2. J. Phys. Chem. C, 2016, 120,27285