The interaction of water with environmentally relevant surfaces


1 Stanford Synchrotron Radiation Laboratory, Menlo Park, CA 94025.
2 Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720.
3 Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720.

Introduction

Probing the coverage and chemical speciation of molecules at surfaces are of fundamental interest in molecular environmental science. The concentration of water and its dissociation fragments at surfaces affect many highly important interfacial chemical processes and there exist no previous quantitative determinations of the coverage of water on clean metal surfaces at near ambient conditions. We have utilized Ambient Pressure Photoelectron Spectroscopy (AP-PES) to study the water/Cu(111) and Cu(110) systems at pressures up to 1 Torr in the temperature range 270-470 K.

Ambient-pressure PES at BL 11.0.2 at the Advanced Light Source

Main obstacle: scattering of electrons in the gas phase

Comparison of water adsorption on clean Cu(110) and Cu(111)

Saturation O coverage (θ = 0.55)

Lower O coverage (θ = 0.22)

Temperature dependence of surface speciation on Cu(110) at 1 torr

Conclusions

• Surprisingly large difference in water chemistry on Cu(110) and Cu(111)

  Cu(110) 5 different species (H2O, OH, and O in different local environments) were observed as a function of pressure and temperature.

  Cu(111) No adsorbate species were observed.

• OH-H2O interaction is stronger than H2O-H2O interaction

  H2O molecules on hydroxylated metal surfaces are more strongly adsorbed than H2O in pure water layer.

• The wettability can be controlled by changing the adsorbed state of the preadsorbed O.

Control of wettability of Cu(111) by coadsorption of oxygen

Discussion: mixed OH+H2O phases on Pt(111)


DFT Calculation using pair potentials


Acknowledgement

This work was supported by the Office of Science, Biological and Environmental Research, Environmental Remediation Sciences Division, US Department of Energy. We would like to thank Ed Wong and Tolek Tyliszczak for their help.