

Abstract Submitted  
for the MAR17 Meeting of  
The American Physical Society

**Molecular-Scale Investigation of Heavy Metal Ions at a Charged Langmuir Monolayer**<sup>1</sup> WILLIAM ROCK, BAOFU QIAO, AHMET UYSAL, Argonne National Laboratory, WEI BU, BINHUA LIN, University of Chicago — Solvent extraction – the surfactant-aided preferential transfer of a species from an aqueous to an organic phase – is an important technique used in heavy and precious metal refining and reprocessing [1]. Solvent extraction requires transfer through an oil/water interface, and interfacial interactions are expected to control transfer kinetics and phase stability, yet these key interactions are poorly understood [2]. Langmuir monolayers with charged headgroups atop concentrated salt solutions containing heavy metal ions act as a model of solvent extraction interfaces; studies of ions at a charged surface are also fundamentally important to many other phenomena including protein solvation, mineral surface chemistry, and electrochemistry. We probe these charged interfaces using a variety of surface-sensitive techniques – vibrational sum frequency generation (VSFG) spectroscopy, x-ray reflectivity (XRR), x-ray fluorescence near total reflection (XFNTR), and grazing incidence diffraction (GID). We integrate experiments with Molecular Dynamics (MD) simulations to uncover the molecular-level interfacial structure. [1] P. Tasker et al., *Comp. Coord. Chem. II*, 2003, 759. [2] W. Rock et al., *Langmuir*, 2016, 32 (44), 11532.

<sup>1</sup>This work is supported by the U.S. DOE, BES, Contract DE-AC02-06CH11357. ChemMatCARS is supported by NSF/CHE-1346572.

William Rock  
Argonne National Laboratory

Date submitted: 11 Nov 2016

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