☒ **Talk** ☐ **Poster**

Pb^{2+} Sorption at the Barite (001)–Water Interface under Hydrothermal Conditions

Peng Yang[a,b], Sang Soo Lee[a], Paul Fenter[a], Andrew G. Stack[c]

[a]*Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439, United States*
[b]*National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY 11973, United States*
[c]*Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, United States*

Author Email: pyang2@bnl.gov

The interactions between ions and ionically bonded minerals play a critical role in governing the fate and transport of ions in natural and engineered systems. These interactions are also central to processes such as mineral dissolution and precipitation, which in turn influence ion mobility. Barite ($BaSO_4$) is an ionically bonded mineral commonly found in hydrothermal vent deposits and is a major scale-forming mineral in oil and gas wells, where hydrothermal conditions can be found. Understanding how metal ions such as Pb^{2+} interact with barite under such conditions is therefore of significant importance. In this study, the sorption behavior of Pb^{2+} on the barite (001) surface at a fixed Pb^{2+} concentration (100 μM) across a range of temperature (25–230 °C) and pressure (15–600 psi) has been examined. Synchrotron-based X-ray crystal truncation rod and resonant anomalous X-ray reflectivity were employed to probe the interface at atomic-scale resolution. The results show that the barite surface initially dissolves as temperature increases to ~100 °C but then recrystallizes at higher temperatures. Despite these structural changes, Pb^{2+} consistently sorbs at the barite-water interface, with overall surface coverage increasing with both temperature and pressure. At temperatures up to 160 °C and pressures up to 300 psi, Pb^{2+} predominantly incorporates into the top atomic layers of the barite. At higher temperatures and pressures, Pb^{2+} is found to both incorporate and adsorb onto the surface. These variations in surface structure and sorption behavior are closely correlated to the temperature and pressure-dependent solubility of barite. Overall, this study demonstrates that under hydrothermal conditions, barite can uptake greater amounts of impurity metal ions such as Pb^{2+}. These findings have important implications for understanding the geochemical fate and transport of contaminants in environments dominated by ionically bonded minerals.