Probing Metal Transport in Ore-forming Fluids Using Molecular Simulations

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Aqueous fluids are an important medium for transporting metals in the Earth's crust and are responsible for the enrichment of ore metals and the formation of many types of magmatic-hydrothermal deposits (porphyry Cu/Mo, skarn, and epithermal deposits). Understanding the nature and thermodynamic properties of ore metals (e.g., Cu, Au, Zn) and various ligand-forming volatile elements (e.g., S, Cl) in magmatic-hydrothermal fluids underpins our knowledge not only the formation of magmatic-hydrothermal deposits and water-rock interactions in geothermal systems, but also of industrial processes such as corrosion in power plants, hydrometallurgy, or material synthesis and catalysis.

This research takes advantage of recent advances in high performance computing to perform first principle Molecular Dynamics (MD) simulations on metal speciation and obtain thermodynamic properties to predict metal solubility in ore-forming systems from dense fluids to vapors. The bulk of our knowledge about metal transport and enrichment in ore-fluids originates from field observations and experimental studies. MD simulation techniques are emerging as a powerful tool for probing the behavior of metals in these systems. In particular, ab initio MD, in which atomic interactions are described using quantum mechanical theory, is now becoming viable for the study of metal speciation and thermodynamics under a wide range of T-P conditions.

Our recent MD simulations provide a realistic estimate of metal (Cu, Au, Zn, and Pd) complexation and solubility in chloride- and sulfur-rich ore-forming fluids over a wide range of temperatures and pressures, at fluid densities ranging from brines to vapors. These MD simulations (1) help to resolve the uncertainty in the interpretation of experimental data—for example, providing a speciation model that was used to successfully reinterpret seemingly inconsistent experimental data for Zn(II) in chloride brines provided much improved capabilities for modeling Zn transport in crustal fluids; and (2) provide estimates of metal speciation in magmatic-hydrothermal ore-forming fluids under conditions important for ore formation (e.g., high temperature; high salinity; low density vapor phase) where experiments are impractical or impossible. Coupled with experiments, in particular in situ spectroscopic studies of the nature and geometry of metal complexes in hydrothermal fluids, MD simulations provide molecular-level insights into the chemical processes responsible for the formation of ore deposits.