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AMASS Consortium

- Portlandite ($\text{Ca}(\text{OH})_2$), hematite (Fe_2O_3), uranyl (UO_2^{2+}) and water are likely to be found in a geological disposal facility (GDF)
- Understanding the mobility of uranyl species is key for determining the viability of a GDF – will uranyl adsorb or incorporate into portlandite and hematite?
- MM, QM and QM/MM studies of uranyl hydroxide complexes in water on portlandite and hematite
- PMF calculations to calculate free energy barriers to adsorption on different material surfaces
- Substitution of U(VI) for Fe(III) to determine how uranium incorporates into iron oxides

