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Evaluation of aqueous speciation of Nd in chloride-bearing solutions by quantum mechanics/molecular mechanics molecular dynamics simulations

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New technologies, particularly those designed to address environmental concerns, and being essential for renewable energy applications (such as wind turbines, solar panels, electric cars, and advanced batteries), have called for a great demand for Rare Earth Elements (REEs) materials. Considering that there is now almost universal agreement that hydrothermal fluids play a significant and in some cases dominant role in the formation of REE ore deposits, it is necessary to understand the mobility/speciation of REE in hydrothermal solutions at a very wide range of conditions.

Ab initio molecular dynamics (AIMD) simulations provide an essential tool permitting to acquire molecular level understanding of the processes occurring in aqueous solutions under different conditions and for the calculation of thermodynamics binding constants, which can not be measured experimentally in some regime. However, due to the steep numerical scaling with respect to the number of atoms and quality of the description of the system, off-the-shelf AIMD methods are currently limited to ~500 atoms and picosecond timescales, which effectively limits the accuracy of the phase-space sampling. Moreover, open-shell nature of REEs causes additional increase in computational time.

In this talk we will discuss promises and pitfalls of approaches that can solve the scaling issue of AIMD, specifically quantum mechanics/molecular mechanics molecular dynamics (QM/MM MD) simulations and Machine-Learned Based AIMD. Preliminary results will be presented for Nd system in chloride-bearing solutions by means of QM/MM MD.