



Showcasing research from X. Wang *et al.*, *Chemical Sciences* and Engineering Division, Argonne National Laboratory, Lemont IL, USA.

Metadynamics investigation of lanthanide solvation free energy landscapes and insights into separations energetics

Lanthanide ion solvation chemistry in nonaqueous phases is key to understanding and developing effective separation processes for these critical materials. We use classical molecular dynamics (MD) simulation with an advanced sampling technique, metadynamics, supplemented by experimental spectroscopy and speciation analysis, to measure lanthanide solvation free energy landscapes. Simulations show how ligand crowding at the metal center can control selectivity, resulting in different extraction trends as observed with conventional extractants.

Credit: UChicago Argonne, LLC, Operator of Argonne National Laboratory.

As featured in:



See Xiaoyu Wang,
Michael J. Servis *et al.*,
Chem. Sci., 2024, **15**, 16494.