Department of Chemistry & Biochemistry

School of Integrated Science and Humanities

Departmental Seminar Announcement

Using theory to guide ligand design for chemical separations of f-block metal ions

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First-principles calculations and computer-aided molecular design of viable host architectures can significantly reduce the efforts in the design of novel ligands for chemical separations of f-block metal ions. In this talk, I will discuss computational methodologies based on density functional theory (DFT) for predictive modeling of complexation behavior of target metal ions and how this knowledge can be used to devise new complexants, extractants, and adsorbent materials. The application areas include separation of adjacent lanthanides, partitioning of minor actinides from high-level waste, and extraction of uranium from seawater. Validation of the theoretical predictions against the experimental data provides the basis for a more detailed investigation of factors controlling affinity and selectivity. The success in rationalizing and predicting binding affinity and selectivity on a molecular level demonstrates the potential of the computational methods for accelerated screening and discovery of more efficient and selective ligands.

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Marine Sciences Building Room 105 (MSB-105) – BBC (via Polycom)

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