M. SANTOSH DAWARE
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donnera un séminaire intitulé

Wealth from Waste: Designing a Task Specific Solvent Extractant Combination

le **mercredi 25 septembre 2019** à **14h00**

en salle Mezzanine

The existing methods for the design of the solvent extractant system is based on a trial and error process. Conventional methods require a huge amount of time and money for design and commercialization. This presentation relates generally to a method and system for rational design of task specific solvent-extractant combinations. For instance, detailed computational chemistry calculations are performed in order to design a solvent extractant combination for the selective separation of a set of target metal ions from each other. These calculations involve the use of ab-initio electronic structure methods to identify the optimal binding configuration of the extractant's functional groups with the target metal ions, followed by using a host designer software to build the extractant molecules by linking the functional groups. Subsequently, aqueous binding free energy of the designed extractant with the metal ion is computed to obtain a measure of its selectivity. Finally, classical molecular simulations together with thermodynamic integration and umbrella sampling is used to predict the partition coefficient and an energy barrier for the transport across the aqueous organic interface, respectively. The most promising task specific solvent-extractant combination is identified using the aqueous selectivity, partition coefficient and energy barrier for transport across the aqueous organic interface. The framework is validated by experiments with known extractant D2EHPA and is used to evaluate its selectivity towards dysprosium over neodymium. The framework is used to design new bishydroxymate type ligands, similar variants of which are synthesized at ICSM.