Quantum Mechanics Basics and Applications in Developing Heavy Element Extractants

Theresa L. Windus

Iowa State University and The Ames Laboratory
Ames, IA 50011

Quantum mechanics as expressed as electronic structure theory is a key player in understanding chemistry and the essential properties of chemical reactions. This talk will give an introduction to the basic underpinnings of electronic structure methods include Hartree-Fock, basis sets and correlation methods. Then the application of these methods and others will be discussed in the context of developing extractants for critical materials. Critical materials are elements that are essential for technological advances, but that are subject to supply disruptions. Many of these critical materials are necessary for clean energy devices such as wind turbines, solar panels and electric vehicles. Of particular interest to the Department of Energy sponsored Critical Materials Institute are lanthanide metals such as neodymium, europium, terbium, and dysprosium. However, these metals can be extremely difficult to separate from one another in the extraction processes and, therefore, new extractants that selectively bind one metal over another are required to make the process more efficient and cost-effective. Towards that end, we are using computer aided molecular design to determine new potential extractants that will cut down on the experimental expense of designing an extractant.