University of Central Florida
Department of Chemistry Seminar Series – Fall Semester 2023
Friday, October 27th, 9:00 am, CB2 105

Computational Science Applications in Separations of Rare Earth Elements and Actinides

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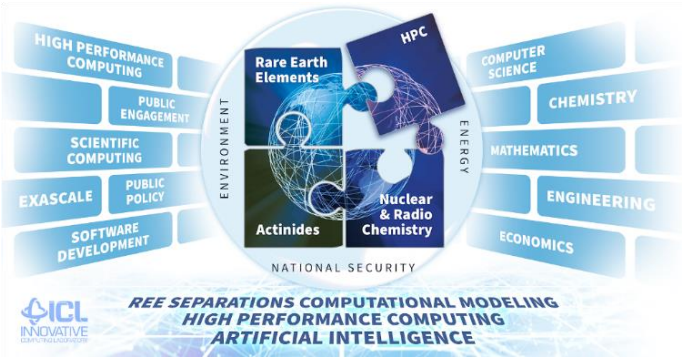
Host: Professor Vasileios Anagnostopoulos

Abstract: Computational science is bolstered by the capabilities of High-Performance Computing (HPC) and data-driven methodologies. Nestled at the crossroads of computer science, mathematics, and domain-specific disciplines, these tools foster a deeper understanding and provide solutions to diverse challenges such as climate change, medical treatments, diagnostics, and technological innovations.

As we transition into the exascale computing era, accurate modeling and predictions concerning the separations of Rare Earth Elements (REEs) and actinides become paramount. Addressing this requires a multidisciplinary approach, particularly in designing software that not only captures the physical nuances of systems containing REEs and actinides but also harnesses the potential of emerging heterogeneous HPC architectures. Moreover, for AI to be effectively applied in the separation of REEs and actinides, there is a need for reliable data sets and refined algorithmic evaluations, especially in predicting binding characteristics.



This presentation aims to shed light on the applications of HPC, data-driven approaches, and AI methodologies in separations pertinent to REEs and actinides. Topics will encompass multidisciplinary strategies in software development, the purification of elements for radiotherapeutics, selective binding techniques for environmental remediation, and the ongoing initiatives within the 'Carbon, Ore, Rare Earth, and Critical Materials (CORE-CM) Project' at the University of Tennessee. We will also explore the collaborative efforts to inform public policy, bringing together researchers, policymakers, and the general public.

Bio: Dr. Deborah Penchoff is the Associate Director of the Innovative Computing Laboratory, and a Research Assistant Professor in the Department of Nuclear Engineering (UTNE) at the University of Tennessee, Knoxville (UTK). She is also a Fellow of the Baker School of Public Policy and Public Affairs, where she serves in the Center for Energy, Transportation and Environmental Policy, and the Center for National Security and Foreign Affairs. She has a PhD in Physical Chemistry and is a graduate from the UTK Interdisciplinary Graduate Minor in Computational Sciences. Penchoff leads the High Performance Computing (HPC) and Artificial Intelligence (AI) efforts in the DOE-NNSA Consortium for Nuclear Forensics, efforts involving AI for environmental remediation, HPC-enabling capabilities for domain sciences, and separations of rare earth elements and actinides, including applications in critical minerals and radiotherapeutics.