Computational Science Applications in Sustainability

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This presentation will highlight computational science applications in areas critical to advancing efforts in sustainability and green economies. Topics will include applications of High Performance Computing (HPC), chemical modeling, data science, and Artificial Intelligence (AI) to areas in environmental remediation and sustainability. Highlights will include optimization of chemical separations involving rare earth elements (REEs) and actinides; binding to transition metals in nuclear forensics applications; and agricultural productivity through biochar utilization.

Current efforts in applications of AI frameworks to predict biochar morphologies' relationship to carbon sequestration and fertilization capabilities will be highlighted. In addition, research progress in HPC-enabling capabilities and computational chemistry methods to develop greener REE separation processes will be discussed as a key contributor to reducing independence of REE sources. Selective binding in broader chemical binding needs will also be discussed, including radiochemical separation in nuclear waste management, and removal of anthropogenic contaminants in environmental remediation.

The AI-driven REACKT (Rare Earth Actinides Constants & logK Thermodynamics) model and applications to selective binding will be highlighted. REACKT is designed to accurately predict reaction characteristics (such as logK values) involving REEs, actinides, and other metals. Building upon advanced algorithms and a comprehensive dataset, REACKT provides reliable estimations that are vital for a range of scientific and industrial applications. Its innovative architecture not only ensures precise predictions but also contributes to a deeper understanding of the complex interactions between these elements and extracting agents – contributing to fundamental understanding of selective chemical binding.