

Faculty Name:

D.R. Nagaraj / Raymond Farinato

Faculty Email:

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Lab:

S3M

Project Title:

Density Functional Theory (DFT) Calculations and Coordination Chemistry of Reagents Used in Separation Science and Their Interaction with Mineral and Solid Surfaces

Description:

Work with graduate students and post-docs to assist in the development of a deep understanding of the coordination chemistry of reagents used in separation science and their interaction with the mineral surface. Adjusting the selectivity in the adsorption of the reagents on a target surface in separation science is governed by the interaction between the reagent molecule and the mineral surface. Coordination chemistry plays a significant role in defining the selectivity in this adsorption and interaction. In this project, various combinations of the reagent-mineral surface will be modeled and the adsorption energy of the system along with other coordination chemistry properties of the system will be calculated via a DFT package. The student researcher will also participate in proposal preparation based on the aforementioned systems of interest for computational allocations.

Location of Research:

Hybrid

of hrs/week:

30

Department/Program:

Earth and Environmental Engineering

Eligibility:

BS, Fourth Year, MS

To apply, please contact:

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