

**Environmental Engineering**

**and Earth Sciences**

**EEES Department Seminar**

**‟** **Exploring the chemistry of uranium dioxide through**

**quantum-mechanical modeling”**

**Presented By**

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<https://clemson.zoom.us/j/5783910968>

**Abstract**

We care about the role of impurities in spent nuclear fuel because of the potential fate and transport of radionuclides in a deep geological repository over time.

America generates 20 % of its electricity from nuclear energy. The material used to power nuclear power plants is uranium dioxide. The fuel is considered “spent nuclear fuel” once the fuel has reached its end of life. The composition of spent nuclear fuel consists of uranium dioxide and impurities such as fission products, activation products, and long-lived transuranic. Understanding these impurities in the fuel matrix is essential because it can influence the properties that govern dissolution. We explore how impurities impact the structural, chemical, and energetic properties of uranium dioxide through quantum-mechanical modeling.

For this presentation, I will discuss in detail about defects in uranium dioxide. Time permitting, I will discuss an interesting alteration product of uranium that is important for repositories under reducing conditions. The goal of this presentation is to show the importance of understanding the chemistry of uranium dioxide and how we achieve this goal through modeling.



***About the speaker:***

Megan Hoover is a Ph.D. student in the Nuclear Environmental Engineering and Sciences group at Clemson University with Dr. Lindsay Shuller-Nickles. She received a BS in Mathematics and MS in Physics from the University of Texas at Arlington.

***Friday, December 4, 2020***

***2:30 PM***

***Online via Zoom***

***“Attendance is mandatory for graduate students enrolled in EES 8610, EES 9610, and GEOL 8510.”***