

# Seminar

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## Institute for Plasma Research

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**Title:** Structural Phase Transition, Defect Formation and Diffusion in Actinide Dioxides: A Theoretical Study  
**Speaker:** Dr. Shilpa Singh  
Gujarat University, Ahmedabad  
**Date:** 11<sup>th</sup> October 2023 (Wednesday)  
**Time:** 03:30 PM  
**Venue:** Seminar Hall, IPR

### Abstract

Actinide dioxides ( $AnO_2$ ) are common nuclear fuels used in nuclear reactors. For safe operation of nuclear reactor, it is very important to understand the properties of these oxides at higher temperature and pressure. The radioactive nature, pyrophorocity, non-stoichiometric behaviour and toxicity make experimental study of these oxides very challenging. However, computational methods have been proved to be an effective complimentary way to investigate the properties of these materials.

There is significant inconsistencies in the reported proeprties such as electronic properties, phase transition pressure, defect formation energy etc. of these oxides. Therefore, I systematically studied the structural phase transiton in these oxide with pressure. I mainly investigated  $ThO_2$ ,  $UO_2$ , and  $PuO_2$ . Nonetheless, the actinide dioxides show similar behaviour under compressive pressure and tensile loading regardless of the existence of 5f electrons. Therefore, the structural phase transition in these oxides is not associated with the electronic response. I also studied the formation and diffusion of point defects and fission gases in these oxides. The defect study validate the stoichiometric behavior of  $ThO_2$  and non-stoichiometric behavior of  $UO_2$  and  $PuO_2$ . The entrapment of *He* and *Xe* suggests that they behave differently inside these nuclear fuel materials. The diffusion of defects shows that, within these oxides, *He* is more mobile than *Xe* and oxygen defects are more mobile than actinide defects. In future, I would like to study the interaction of plasma with oxides.

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