Seminar Title:

"Exploiting Epitaxial Strain and Magnetocrystalline Anisotropy in Double Perovskite Oxides for Advanced Functional Applications"

By Dr. Paresh Chandra Rout, KAUST, KSA.

Abstract:

Transition metal double perovskite oxides [1], characterized by the formula $A_2BB'O_6$ (where A is an alkaline or rare-earth atom and B/B' is a 3*d*/5*d* transition metal atom), have attracted significant attention in the field of room-temperature spintronics. However, challenges such as low critical temperature, low magnetic moments, and spin frustration have posed obstacles to their practical applications. In this talk, I will present my recent research employing density functional theory and Monte Carlo simulations to address these challenges in three specific compounds: Sr_2FeOsO_6, Ca_2FeOsO_6, and Lu_2NiIrO_6. Firstly, I will demonstrate the effectiveness of epitaxial strain in suppressing spin frustration and enhancing the critical temperature in Sr_2FeOsO_6, facilitating its utilization in room-temperature spintronics applications [2]. Additionally, I will discuss the influence of epitaxial strain on Ca_2FeOsO_6, which unveils a strain-induced monoclinic structure and antiferromagnetic phase transition. By controlling the strain, I successfully manipulated the critical temperature of ferrimagnetic ordering and enhanced the spin coherence length, resulting in the establishment of a rich phase diagram [3]. Notably, Ca_2FeOsO_6 exhibits a direct bandgap with electron-hole separation in two distinct magnetic sublattices, offering promising prospects for high-efficiency solar cells [3]. Moreover, I will present the intriguing properties of the Ca_2FeOsO_6/Sr_2FeOsO_6 superlattice, characterized by hybrid-improper ferroelectricity and intrinsic ferrimagnetism. These features hold potential for high-performance solar cells [4]. Furthermore, my research reveals the presence of giant coercivity in Lu_2NiIrO_6, driven by spin-orbit coupling and structural distortions, highlighting its suitability for spintronics applications [5]. Collectively, these findings shed light on the versatility of double perovskite oxides for diverse functional applications. The knowledge gained from this work contributes to the development of novel materials and paves the way for future advancements in spintronics and energy-related technologies.

References:

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3. Paresh C. Rout and Udo Schwingenschlögl, Advanced Science 9, 2106037, 2022.
4. Paresh C. Rout and Udo Schwingenschlögl, Phys. Rev. B 107, 094419, 2023.
5. Paresh C. Rout and Udo Schwingenschlögl, Nano Letters 21, 6807−6812, 2021.