

Title: Computational Materials Design for Energy and Environmental Applications

Abstract: The key critical challenges related to climate change and energy security could be solved if we can find the champion materials to catalyse the energy intensive chemical processes, and build sustainable and environment friendly devices. With this aim in mind, my research leverages a unique combination of leading-edge computational techniques and multidisciplinary approach for designing next-generation materials with unprecedented physical and chemical properties. Materials specifically crucial for catalyzing energyintensive chemical processes (such as ammonia synthesis and CO₂ reduction/conversion), and optimizing fuel cell devices are targeted in my research. In this context, I will present an overview of my most recent research conducted at I2CNER and my future research plans.