ACCMS-Global Research Center
SRMIST, Chennai India

Webinar #28

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Title: Advances and Challenges in DFT-based Design of Energy Materials for Climate Change Mitigation

Registration link: https://tinyurl.com/3w7w9n2r
****Zoom details will be shared with the registered participants***

Short biography

Prof. Siriporn Jungsuttiwong received her B.S. degree in Chemistry from Khon Kaen University in 1994 and PhD degree in Chemistry in 2005 from Kasetsart University. She then became a lecturer in the Department of Chemistry, Ubon Ratchathani University in 2005. She was promoted to professor in 2018. Her research interests focus on Computational and Theoretical Chemistry, specifically on developing new catalysts and adsorbents for air treatment and hydrogen storage. She is also dedicated to advancing catalysts for the conversion of CO_2 into valuable products, contributing to the creation of sustainable energy materials and batteries. Her innovative research not only addresses critical environmental challenges but also drives advancements in nanostructure materials, aiming for a net-zero, climate-resilient future, especially in energy applications.

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Abstract

The growing worldwide energy needs call for developing novel materials for energy applications. The use of ab initio density functional theory (DFT) calculations is crucial in understanding and predicting the properties of materials at the molecular level, thereby playing a crucial role in the design of energy materials. Rapid advancements in computing technology, along with the evolution of computational methodologies, have improved the predictive accuracy of DFT-based calculations. The aim of this perspective is to introduce the advances in DFT calculations which accelerate energy materials design. Initially, we highlight the DFT techniques that enable precise simulations of essential properties of energy materials. Subsequently, we provide examples illustrating how these advancements have enabled the discovery of new energy materials, including those for battery applications. Finally, we discuss the existing challenges and outline future research directions in the computational design of energy materials, emphasizing their significance in meeting both current and future energy challenges.

Keywords: Climate change; Energy materials; Catalyst; DFT

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