Computational Insights and Experimental Integration in Energy Materials: The Role of DFT in Sustainable Energy Solutions

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Abstract:

The rising global energy demand drives the need for innovative materials for sustainable energy applications. Ab initio density functional theory (DFT) calculations have emerged as a powerful tool for understanding and predicting material properties at the molecular level, significantly influencing the design of energy materials. This talk explores recent advancements in DFT methodologies and their integration with experimental insights, highlighting their role in accelerating energy material innovation. Key DFT techniques that enable precise simulations of critical material properties will be introduced. Case studies will illustrate breakthroughs in energy material discovery, particularly for battery technologies. Finally, the talk will address current challenges and propose future directions in computational and experimental collaborations, emphasizing their importance in tackling present and future energy challenges.

Prof. Siriporn Jungsuttiwong

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 for the conversion of CO2 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.