Title: Nanomaterials for Energy, Electronics and Environmental Applications: Contribution from Theoretical Modelling toward Rational Design

Aijun Du

School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology, Science and Engineering Faculty, QLD 4001, Brisbane, Australia

ABSTRACT

Nanoscale material is difficult to manipulate and characterize experimentally because of tiny size. Its properties are in principle determined by its electronic structure. Now first-principles calculations are able to realistically address fundamental questions of structure, stability, adsorption, chemical reaction and electronic properties in nanoscale materials, providing a powerful complement to experimental synthesis and characterization and facilitating the material design process by shedding light “from the bottom up".

My research in Australia aims to provide in-depth understanding of material properties at atomic/molecular level and develop novel strategies to manipulate the electronic structure of nanomaterials through advanced theoretical modelling in close interaction with the active experimental program. In this talk, I will present our key research findings in recent years to show how theoretical modelling can contribute to the rational design of nanoscale materials with potential applications in hydrogen storage, fuel cell, hydrogen purification, photovoltaic and photocatalysis, CO_2 capture and nanoelectronics etc.