Integrated Materials Design Centre Seminar

Jointly Hosted with UNSW School of Chemistry

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Computer-Aided Materials Design

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Date: **Thursday, 10th September 2015**
Time: **11:00 am – 12.00 pm**
Venue: Chemistry Building seminar room G05
Dalton Building (F12)

Abstract

Due to the development of high performance clusters (HPC), computer-aided materials design (CAMD) has emerged as a powerful approach for the development of new materials. In this talk, I will introduce the strategy and capacity of the Monash CAMD group. Several examples will be presented to demonstrate the power of CAMD. GPU technology and reactive molecular dynamics have been employed to study large systems involved in electrochemical and photocatalytic reactions. And time-dependent density functional theory is also employed to study ultrafast charge transfer in photocatalysis. Challenges and opportunities from CAMD have been discussed.

Biography

Dr Chenghua Sun obtained his PhD from Chinese Academy of Sciences in 2007 and joined the University of Queensland (UQ) as a postdoctoral fellow with Prof. Sean Smith and Prof. Max Lu. As a research fellow, Dr Sun worked in UQ from 2007-2013 and visited Royal Institute of Technology (Sweden), Princeton University and Harvard University as visiting postdoctoral fellow. Dr Sun joined the School of Chemistry, Monash University as a lecturer in 2013 and worked as ARC Future Fellow from 2014. Dr Sun is a computational chemist, working on computer-aided materials design, particularly the development of novel materials for clean energy and environment. Dr Sun has published more than 100 peer-review papers, including Nature, J. Am. Chem. Soc., Angew Chem., Adv. Func. Mater., etc., leading to 5400 citations.