NECEM SEMINAR: "Multiscale modelling aided materials design for energy conversion and storage"

Dr Qiong Cai, University of Surrey

14:00pm-15:00pm, Wednesday 15th May 2019

Lecture Theatre 1.75, Bedson Building, Newcastle University

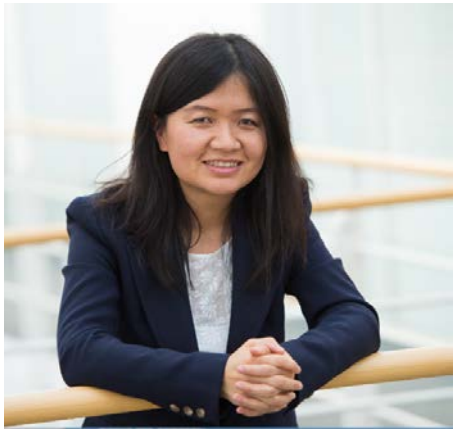
Refreshments available after the seminar

Abstract

"Multiscale modelling aided materials design for energy conversion and storage"

Materials are at the heart of the enabling technologies for energy conversion and storage. Understanding the materials properties and performance relation is a first step towards designing better materials for improved performance, which often requires the assistance of models. This talk will introduce our endeavour to develop the modelling capability at multiple length scales, including: (1) a recently developed 3D microstructure modelling framework based on lattice Boltzmann method, to underpin the multi-physics phenomenon (e.g. multiphase flow) and chemical/electrochemical performance, in relation to materials structure/properties, exemplified by electrode design applications for proton exchange membrane fuel cells, redox flow batteries and lithium-ion batteries. (2) molecular models to reveal the impact of the atomic features of electrode materials on battery performance, using sodium ion battery anode as an example; (3) first principle simulations for developing advanced catalysts for CO2 conversion and hydrogen production. Challenges in multi-scale modelling and opportunities for multidisciplinary collaborations will also be discussed.

Biography



Dr Qiong Cai is a senior lecturer in Chemical Engineering at University of Surrey. Prior to joining Surrey, she was a research associate at Imperial College London where she led the Modelling and Simulation workpackage within a four-year EU FP7 funded project on hydrogen production using solid oxide electrolysers. Her education background include a PhD degree in Chemical Engineering from University of Edinburgh (UK) and a MEng degree in Materials Science and Engineering from Tsinghua University (China).

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She has been researching actively at the interface of materials science and electrochemical engineering. Her current research focuses on multi-scale materials design for energy conversion and storage. She has successfully delivered three EPSRC funded projects as the PI, on Na-ion batteries, polymer membrane fuel cells and capacitive deionization respectively. She has collaborated widely across disciplines and across institutions. She is the Co-I of a collaborative Surrey-NPL (National Physical Laboratory) project on cathode design for lithium-air batteries, the Co-I for a three-year £1.2 million EPSRC funded project in collaboration with Queen Mary University of London and Imperial College London, in which she leads the work-package on multiscale materials modelling. Her current research group consist of 2 postdocs and 5 PhD students. She is on the Scientific Board of the H2FC SUPERGEN Hub, the Scientific Board of the Energy Storage SUPERGEN Hub, and a member of the EPRSC peer review college. She has also been an active referee for a number of international journals including *Journal of Power Sources*, *Electrochimica Acta*, *International Journal of Hydrogen Energy, etc.*

Location
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