

Computational Screening of Inorganic Solid-State Electrolytes for Lithium Batteries**Speaker:** Dai Ruoyu

Department of Materials Science and Engineering, Engineering, NUS, Singapore

Date: 19th Sep 2019, Thursday
Time: 3:00 to 3:30 pm
Venue: EA-06-03**Abstract**

Novel solid electrolytes with their high ionic conductivities and commendable stability have been considered as a promising way to improve the performance of batteries. With Inorganic Crystal Structure Database (ICSD) of 210000 structures, many reported inorganic materials are yet to be explored for their possibility as ion conductors. *SoftBV*, a software designed in the group based on bond valence theory is developed further and used to assess the migration barrier and structural stability of a wide range of potential ionic conductors. For shortlisted materials migration pathways are analyzed more in detail to better understand the ion transport mechanism of the materials. Selected materials have been synthesized and characterized to help improve the computational predictions and strive to make substantial steps on the realization of novel fast ionic conductors.

Dai Ruoyu received his bachelor's degree in Department of Materials and Engineering from National University of Singapore. He is now a PhD candidate in Department of MSE under A/P Stefan Adams. His current research mainly focuses on the lithium ion conductors and computational screening of solid-state ionic conductors.

ALL ARE WELCOME!

Host: A/P Xue Junmin