The 116th GREEN Seminar

Computational Study of Materials and Fundamental Processes for Energy Conversion and Storage

Chair: Dr. Denis Yu(GREEN)

Prof. Patrick Sit

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Density functional theory (DFT) techniques have been powerful tools to provide atomic-scale understanding and realistic prediction of materials properties thanks to the ever-increasing computer power, and the development of more efficient and accurate methodologies. In this talk, I will discuss our works in methodology development and examples of the study of nanoscale processes important in energy applications. In particular, I will present the development of the oxidation-state constrained DFT (OS-CDFT) technique to study charge transfer/polaron hopping processes in transition metal oxides. The technique targets specifically the oxidation states of transition metal ions which is particular useful for the study of electron transfer problems. Moreover, I will also highlight our simulation studies of novel processes in battery materials and catalysis for energy conversion and storage.

Venue: Auditorium, 1F, NanoGREEN/WPI-MANA Bldg., Namiki-site

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