



The Hong Kong University of Science and Technology
Seminar on Scientific Computation Concentration



Computational Materials Science and Sustainability

By
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Abstract

Computational methods have grown to be powerful tools to understand, predict, and design advanced materials to achieve a sustainable environment and provide clean energy to power our planet. In this talk we will introduce some recent development in computational materials science with a focus on the key role of density functional theory (DFT) and its implementations in high performance computer codes. The applications of DFT based methods to sustainable development, e.g., water science, deep carbon cycle, and clean energy will be showed and the challenges will be discussed.

Date: 6 October 2017, Friday

Time: 3:00p.m. - 4:00p.m.

***Venue: Room 2406, Academic Building
(near lifts 17&18), HKUST***

All are welcome!