ACCMS-Global Research Center
SRMIST, Chennai India
Webinar #13

Prof. Yuan Ping Feng

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Title: Computation, Database and Discovery of 2D Materials

27th October 2022, 11.30 am – 1.00 pm IST

Registration link: https://tinyurl.com/5yhzehww

Biography

Prof. Yuan Ping Feng has been a faculty member of Department of Physics at the National University of Singapore (NUS) since 1990. He joined NUS following a 3 year postdoctoral stint at Purdue University. His research interest is in computational condensed matter & materials physics, focusing mainly on the understanding of fundamental properties of materials for advanced technologies, and prediction of new materials based on ab initio electronic structure calculations and materials genomic approach. Over the years, his group has studied various materials including structures, properties and applications of two-dimensional materials, dilute magnetic semiconductors, graphene spintronics, topological insulators, high-k materials, semiconductor and metal surfaces and interfaces, materials for magnetic data storage, etc. He has an established a track record in collaboration with experimentalists. He is a Fellow of American Physical Society (since 2012), and Fellow of Institute of Physics, Singapore (since 2007). He has received several awards like Institute of Physics Singapore President's Medal (2017), NUS Excellent Teacher Award, Faculty of Science Teaching Excellence Awards and so on. He has authored/co-authored close to 600 scientific papers in international refereed journals and one book with the citations of 29689 and h-index -84.

Abstract

Recently, materials Genome approach which integrates computational, data analytics and experimental research has emerged as a new paradigm for discovery of new materials. In this talk, besides an overview on this new paradigm and an outlook for the future, I will focus on our recent work in developing a materials genome for two-dimensional (2D) materials. 2D materials have attracted tremendous amount of interest because their unique properties are expected to lead to new technologies. In an effort of systematic 2D materials discovery, we have been using both the top-down and the bottom-up approaches to generate 2D structures. On one hand, monolayer structures are theoretically exfoliated from layered three-dimensional structures by a topology-based algorithm. On the other hand, new 2D materials are systematically generated by chemical substitution of elements in known 2D compounds by similar elements. High throughput first-principles calculations are carried out to study their basic properties. The database, 2DMatPedia, is publicly available (http://www.2dmatpedia.org/) and provides a good starting point for further material screening, data mining, data analysis and artificial intelligence applications. A few materials design examples will be discussed, including high throughput screening of 2D materials for 2D magnetic electrodes, high-throughput screening of 2D materials for hydrogen evolution and nitrogen fixation, high throughput computational screening of vertical 2D van der Waals heterostructures for high-efficiency excitonic solar cells, etc.

Panelist

Prof. Kwang-Ryeol Lee
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Zoom meeting details will be shared with the registered participants

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