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The Chinese University of Hong Kong
Department of Chemistry
Research Seminar Series

Speaker: Professor Xin Xu
Department of Chemistry
Fudan University

Title: Towards the Accurate Yet Efficient Molecular Modelling of Large Systems from First Principles

Date: November 23, 2018 (Friday)

Time: 3:30 p.m.

Venue: L1, Science Centre

<< Abstract >>

Today, there is a growing demand for theoretical interpretations of ever-complex processes involving ever-larger systems with ever-greater precision. However, the cost of accurate quantum mechanical methods usually scales unfavorably with the system size, which impedes the realization of such goals. Therefore, development of efficient methods capable of accurately describing complex processes involving large systems, such as catalysis, protein folding and others, is a subject of great interest. In this talk, I will present some of the recent works in my group. Emphases will be laid on the development of a new generation density functional for accuracy and the extension of the well-established ONIOM model for complexity, while the combination of both opens up new possibilities for new applications.

Short bio and achievements:

Prof. Xu, Changjiang Professor of Fudan University, is a world-renowned computational chemist. He is a pioneer in the development of Density Functional Theory in quantum chemistry. In particular, the double-hybrid density functional developed in his group is a very efficient functional for large systems. Prof. Xu has won numerous awards including the Changjiang Professorship, National Natural Science Foundation for Outstanding Young Scientists, and Fok Ying Tung Foundation Reward Fund. He currently serves on the editorial board for Theoretical Chemistry Accounts.

ALL ARE WELCOME

Contact Person:
Prof. Steve Y.L. Tse