For favour of Posting

THE HONG KONG UNIVERSITY OF SCIENCE & TECHNOLOGY

Department of Mathematics

SEMINAR ON APPLIED MATHEMATICS

Numerical methods in density functional theory

By

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Abstract

Density functional theory is one of the most successful approximate models in electronic structure calculations. In this talk, our recent works in developing numerical methods for Kohn-Sham density functional theory will be introduced. The framework of the numerical methods is built based on finite element methods. Towards the efficiency, mesh adaptivity, acceleration of self-consistent field iteration, fast solver for Hartree potential, as well as efficient LOBPCG eigensolver will be introduced in detail. In addition, the effort for the orthogonalization-free method will also be described. Numerical results will be demonstrated to show the effectiveness of our method.

Date : 6 July 2023 (Thursday)
Time : 10:00am – 11:00am
Venue : Room 4502 (Lifts 25/26)

All are Welcome!