

Department of Mathematics  
City University of Hong Kong

## Colloquium

Organised by Prof. F. Cucker and Prof. M. Ismail

### Finite Element Approximations in Electronic Structure Calculations

by

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**Abstract** : In this presentation, we will talk about finite element approximations in first-principles electronic structure calculations. We will report several numerical experiments in ground state energy calculations of typical molecular systems, which show that the finite element approach is efficient. This presentation is based on some joint works with Huajie Chen, Xiaoying Dai, Xingyu Gao, Xingao Gong, Lianhua He, Linhua Shen, Zhang Yang, and Dier Zhang.

**Date** : 3 November 2010 (Wednesday)  
**Time** : 4:30pm – 5:30pm  
**Venue** : Room B6605 (College Conference Room)  
Blue Zone, Level 6  
Academic Building  
City University of Hong Kong

(Tea, coffee and cookies will be provided at the College Conference Room in B6605 before the colloquium from 4:00 to 4:30pm. Please come and join us.)

**\*\* All interested are welcome \*\***

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