Physics Pre-Symposium Lecture

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Computational Materials Science by RESCU - a KS-DFT method for solving thousands of atoms

A major stumbling block for solving realistic materials problems is the lack of a first principles method that can accurately, efficiently and comfortably calculate condensed phase materials comprising thousands of atoms. Solving large systems is necessary when dealing with materials physics involving interfaces, surfaces, dilute impurities, grain boundaries, dislocations, magnetic domains, solvents, bio-materials etc.. Well known software of Kohn–Sham density functional theory (KS-DFT) can typically solve problems at a few hundred atoms level. For very large systems, further approximations are typically applied at the expense of accuracy. **In this talk** I will discuss our effort in developing a powerful general-purpose KS-DFT solver called RESCU1. We demonstrate that RESCU can compute electronic structure for systems comprising many thousands of atoms on modest computer resources, for metals, semiconductors, insulators, DNA-in-water, Moire patterns in 2D heterjunction materials, dilute doped III-nitrides, etc.. For these problems and up to 14,000 atoms, RESCU converges KS-DFT in a few to ten wall-clock hours. RESCU achieves high efficiency without compromising accuracy. I shall discuss the novel computational mathematics behind the efficiency gain1, and present several materials physics examples solved by RESCU.

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**BIO:** Born in the city of ShengYang, Liaoning Province, China, a loooooooooooong time ago. Grow up in the city of Chengdu, Sichuan (eat very hot food). Spent three years in rice fields after high school, lived in a hut on top of my little hill overlooking a small valley. No electricity, no running water, life was tough but I did not notice, managed to generate tons of fun there. 1976 (precisely March, 1977), started undergrad at the Sichuan Normal University to become a high school teacher. 1980, had the fortune to pass the first national CUSPEA exam. 1981, graduate student at University of Pittsburgh (Pitt), obtained PhD under Professor David Jasnow. 1987, postdoc under Prof. Jim Gunton at Temple University in Philadelphia. 1989, came to Montreal to work with Prof. Martin Grant at McGill. 1990, joined the Physics faculty at McGill. It has been 27 years of service at McGill University in 2016.

I had the fortune to work with large number of outstanding graduate students and postdoc fellows.

**Election to Prestigious Memberships**

- 2004, elected to Fellow of the American Physical Society.
- 2007, elected to Fellow of the Royal Society of Canada.

**Major Research Awards**

- Killam Research Fellowship Award, 2004-2006.
- CAP-CRM Prize for Theoretical and Mathematical Physics, 2009