NANYANG TECHNOLOGICAL UNIVERSITY

CBC SEMINAR ANNOUNCEMENT

Professor Chen Guanhua
University of Hong Kong

Time-Dependent Density-Functional Theory for Open Systems

First-principles methods have been limited to the isolated systems. It would thus be a good idea to extend them to the open systems where the number of electrons and energy are no longer conserved. We have proven that the electron density function of a subsystem determines uniquely the electron density or electronic properties of the entire system, which is the so-called Holographic Electron Density Theorem. Based on this, a rigorous first-principles method is sought for the open system, and it needs the electron density of the system of interest. A single-particle Liouville-von Neumann equation is proposed and developed for such a theory, and has been used to simulate from first-principles the transient current through electronic devices.

Date:	**2nd August 2012 (Thursday)**
Time:	**2:30pm – 4:00pm**
Venue:	**NTU SPMS CBC Building Level 2, Conference Room**
Host:	**Dr Hajime Hirao**