Joint CQSE and CASTS Special Seminar

Special Seminar
Dec. 10, 2015 (Thursday)

TIME Dec. 10, 2015, 14:30 ~ 15:30
TITLE How density functional theory argumentation can help designing new perturbation methods
SPEAKER Prof. Andreas Savin
Laboratoire de Chimie Théorique, CNRS and UPMC Sorbonne Universités
PLACE Rm716, CCMS & New Physics Building, NTU

Abstract

After recalling the basic ideas of density functional approximations, it will be shown that density functional theory allows more flexibility than in the widely used Kohn-Sham method, without a significant increase of complexity:

1) typical quantum mechanical effects can be treated explicitly, using multi-determinant wave functions for model Hamiltonians, and using density functional corrections can be introduced to obtain the energy of the physical system,

2) double counting (often showing up in combined methods) can be avoided.

This approach builds a bridge starting from approximate Kohn-Sham calculations, reaching in a systematic way exact wave function results.

Next, it will be shown how to replace in the approach above density functionals, and use systematically improvable numerical techniques instead. The principle of this "energy extrapolation" is explained, and some numerical examples are given, but now fast implementation of the idea exists at the present moment.