

## Theoretical Chemistry Colloquium

**March 14, 2014 (Fri), 16:00-17:00**

**RCMS, 2<sup>nd</sup> floor, Chemistry Gallery**

### *Development of the systematic molecular fragmentation method based on DFTB*



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**Abstract:** *Systematic Molecular Fragmentation (SMF) is a well-known method that approximates the total electronic energy of a molecule as a sum of energies of fragments in the molecule. Several implementations<sup>1,2</sup> exist as well as several correction schemes<sup>3</sup> improve the accuracy of the method by taking into account interactions between distant, "non-bonded", parts of the molecule. Such calculation schemes are often used to approximate energies of moderately sized molecules (20-100 atoms) using high levels of ab initio theory, such as MPn and CCSD(T), where they reduce the prohibitive,  $N^5$  or  $N^7$  scaling to approximately linear ( $N^1$ ). As the many fragment calculations can be carried out entirely independently, molecular fragmentation schemes represent an ideal approach to carrying out large calculations on PC-clusters. With this in mind, we take the SMF approach and adapt it to the calculation of truly huge (2,000 - 10,000+ atoms) molecules using the Density Functional Tight Binding (DFTB) method.*

**References:**

1. Deev, V. and Collins, M. A. *J Chem. Phys.* **122** 154102 (2005)
2. He, X. and Zhang, J. Z. *J Chem. Phys.* **124** 184703 (2006)
3. Addicoat, M.A. and Collins, M. A. *J Chem. Phys.* **131** 104103 (2009)



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