Theoretical Chemistry Colloquium

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

RCMS, 2nd 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[1,2] exist as well as several correction schemes[3] 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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