RCMS Research Center for Materials Science, Nagoya University

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Platform: Nano-Energy

Theoretical Chemistry Colloquium

December 8, 2014 (Mon), 16:00-17:00

RCMS, 2nd floor, Chemistry Gallery

Range separated functionals in the density functional based tight-binding method: Formalism, implementation and first results

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Abstract: A generalization of the density functional based tight-binding method (DFTB) for the use with range-separated exchange-correlation functionals is presented [1]. It is based on the generalized Kohn-Sham (GKS) formalism and employs the density matrix as basic variable in the expansion of the energy functional, in contrast to the traditional DFTB scheme. We will discuss details of a numerically efficient implementation and present first results on quasiparticle gaps in organic molecules and the extension of bipolaronic defects in polythiophenes.

[1] T.A. Niehaus and F. Della Salla "Range-separated functionals in the density functional based tight-binding method: Formalism", Phys. Stat. Sol. B, vol. 249, pp. 237, 2012.

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