RCMS Research Center for Materials Science, Nagoya University

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Platform: Nano-Energy

Theoretical Chemistry Colloquium

January 9, 2015 (Fri), 13:00-14:00

RCMS, 2nd floor, Chemistry Gallery

Density-functional based tight-binding method for exotic systems

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Abstract: The semi-empirical density-functional tight-binding (DFTB) method is particularly well know for its applications to organic and biomolecular systems, as a fast replacement for density functional theory. Instead I will discuss some of the more unusual systems for which DFTB has been recently extended to treat, including cases where spin-orbit or electron correlation become important, or where the geometry of the system is more exotic (irrational helices, or weak magnetic fields for periodic boundaries).

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