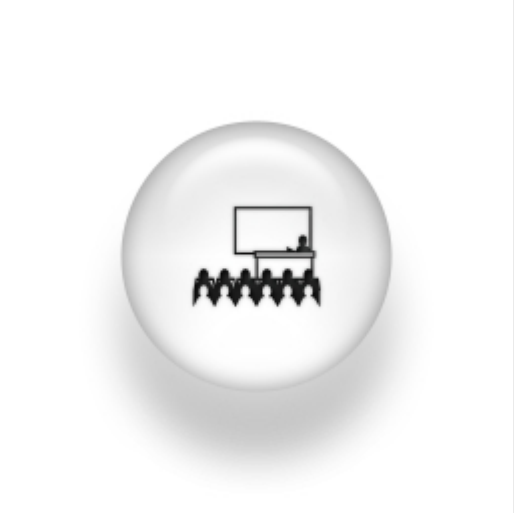
Density Functional Theory - OpenMX

Thursday, 7 April 2011, 12:00-13.00



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ABSTRACT:
During the last three decades continuous efforts have been devoted to extend applicability of the density functional theory (DFT) to large-scale systems, leading to realization of more realistic simulations close to experimental conditions. In this talk, I will introduce our recent developments of low-order scaling methods for eigenvalue problem and evaluation of exact exchange energy towards the direction [1-5]. It is demonstrated that a linear-scaling Krylov subspace method [1], combined with effective screening medium (ESM) method [6], enables us to simulate a bias induced chemical reaction in lithium battery. Moreover, a numerically exact low-order scaling method is presented [2,3], which directly evaluates selected elements of density matrix using a nested dissection approach. Finally, an exchange functional by a range-separated exchange hole, whose computational cost is linear-scaling, is proposed to calculate the exact exchange energy [4]. I will also summarize the OpenMX project [5] in an east Asian community to develop a platform for large-scale DFT simulations.
[1] T. Ozaki, PRB 74, 245101 (2006).
[2] T. Ozaki, PRB 75, 035123 (2007).
[3] T. Ozaki, PRB 82, 075131 (2010).
[4] M. Toyoda and T. Ozaki, PRA, in press.
[5] http://www.openmx-square.org/
[6] M. Otani and O. Sugino, PRB 73, 115407 (2006).