

# Large-scale electronic structure calculation and its application

Takeo Hoshi<sup>1</sup>, Ryu Takayama<sup>1,2</sup> and Takeo Fujiwara<sup>1</sup>

<sup>1</sup> Department of Applied Physics, University of Tokyo, <sup>2</sup> ACT-JST(JST)

## abstract

The present talk is devoted to constructing the methods in large-scale electronic structure calculations and their application to nanoscale materials [1-4].

In general, a physical quantity  $\langle \hat{X} \rangle$  is given as

$$\langle \hat{X} \rangle = \sum_k^{\text{occ.}} \langle \phi_k^{(\text{eig})} | \hat{X} | \phi_k^{(\text{eig})} \rangle = \text{Tr}[\hat{\rho} \hat{X}] \quad (1)$$

with occupied eigen states  $\{\phi_k^{(\text{eig})}\}$  or the one-body density matrix  $\hat{\rho}$

$$\hat{\rho} \equiv \sum_k^{\text{occ.}} |\phi_k^{(\text{eig})}\rangle \langle \phi_k^{(\text{eig})}|. \quad (2)$$

Since the calculation of eigen states gives a severe computational cost, the essential methodology for large-scale calculations is how to obtain the density matrix  $\hat{\rho}$  without calculating eigen states. The practical solver methods are based on quantum mechanical equations of generalized Wannier state or Green function, instead of eigen state. A hybrid scheme is also formulated within quantum mechanics by dividing the occupied Hilbert space. The basic idea is to divide the density matrix into two subsystems ( $\hat{\rho} = \hat{\rho}_A + \hat{\rho}_B$ ) with respect to one-electron states and to calculate the resultant subsystems,  $\hat{\rho}_A$  and  $\hat{\rho}_B$ , using different solver methods. The fundamental equation for a subsystem,  $\hat{\rho}_A$ , is derived in the form of the commutation relation ( $[\hat{\rho}_A, \hat{H}_{\text{map}}^{(A)}] = 0$ ) with a mapped Hamiltonian  $\hat{H}_{\text{map}}^{(A)}$ . The practical calculations are carried out within tight-binding Hamiltonian. Though the applicability is limited, its parameter theory reproduces systematically several *ab initio* results among different elements or phases, because the tight-binding formulation is universal within the scaled length and energy units.

Test calculations with upto  $10^6$  atoms are done by a standard workstation and with upto  $10^7$  atoms by a parallel computation. As a practical nanoscale application, the molecular dynamics simulation is performed for fracture of nanocrystalline silicon [2].

Recently the concept ‘multiscale mechanics’ is focused as the seamless theoretical connection of material simulation methods among the three principles of mechanics; quantum mechanics (for electron systems), classical mechanics, and continuum mechanics. The present work gives a guiding principle and a typical example for the concept, which is carried out by simplifying the total energy with respect to quantum mechanical freedoms of electrons.

[1] T. Hoshi and T. Fujiwara, JPSJ **69**, 3773 (2000). [2] T. Hoshi and T. Fujiwara, cond-mat/0210366, to appear in JPSJ **72**, Vol. 10 (2003). [3] M. Geshi, T. Hoshi and T. Fujiwara, cond-mat/0306461. [4] R. Takayama, T. Hoshi and T. Fujiwara, in this workshop.