Computational Physics Course

Learn to use software packages

Final day: Large-scale calculation

PDF

Introduction

The total energy is given by

E=\sum e_i -EH + (exchange correlation contribution) (1)

within the Kohn-Sham (KS) approach to the density functional theory (DFT). Note the first term on the right-hand side of Eq. (1). It is a sum of the Kohn-Sham eigenvalues , which are obtained by diagonalizing the Kohn-Sham Hamiltonian . The diagonalization requires computational time that grows as with the number of basis functions , hampering thereby large-scale calculation. It is difficult to handle over 10,000 atoms even with the modern supercomputers. 10,000 atoms are typically contained in a computational cell of spatial dimension several nanometers. (Consider, for example, the crystalline silicon where 8 atoms are contained in a cell of 0.5 nm3) However, the frontier of research, such as interfaces or nanomaterials, often requires even larger-scale calculation. It is therefore important to find a way to do the calculation without diagonalization. In this lecture, we focus only on the first term in the right-hand side of Eq. (1), so that we share the problem with researchers focusing on the tight-binding calculation.

Having learned DFT, let us move to learning program packages. We begin by learning Quantum Espresso

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