n's function approach for calculating total energies in molecules a

Table of Contents

Green's function approach for calculating total energies in molecules and solids.

T. Miyake[1], F. Aryasetiawan[2], and K. Terakura[3],

[1]*Tokyo Institute of Technology, 2−12−1 Oh−Okayama, Meguro−ku, Tokyo 152−8551, Japan*

[2]*JRCAT−ATP, 1−1−4 Higashi, Tsukuba, Ibaraki 305−0046, Japan*

[3]*JRCAT−NAIR, 1−1−4 Higashi, Tsukuba, Ibaraki 305−8562, Japan*

Traditionally, many−body Green's function is used to calculate quasiparticle energies and one−particle excitation spectra. However, it is also known that total energies can be obtained from the Green function. This possibility has recently received a growing attention because it may have a potential as an alternative method to currently available techniques, with the same level of accuracy as that of the Quantum Monte Carlo method but with much less computational time, as has been shown by recent works on the electron gas.

Here we consider two formulations for calculating total energies. The first is based on the Galitskii−Migdal formula [1] where the main ingredient is the one−particle spectral function (density of states). We recently proposed a model spectral function [2] where the parameters of the model can be calculated from first−principles using, e.g, the GW approximation. This scheme has been tested on the electron gas and has successfully reproduced the Quantum Monte Carlo data for the total energy. We have also tested the scheme on real systems by calculating the equilibrium lattice constants of Na and Al with encouraging results.

The second approach is based on the well−known formula due to Luttinger and Ward [3]. Although it is more complicated than the Galitskii−Migdal formula, it has the advantage of being variational with respect to the one−particle Green's function. Application of this method to equilibrium lattice constant of Na has yielded a promising result.

[1]

V. M. Galitskii and A. B. Migdal, Sov. Phys. JETP **139**, 96 (1958).

[2]

B. Holm and F. Aryasetiawan, Phys. Rev. B **62**, 4858 (2000).

[3]

J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).