

Investigation on transport properties in nanostructures with contacts

Abstract

The transport properties of nanostructures coupled with contacts were studied theoretically by using Non-equilibrium Green's functions method. Physical quantities, such as density of states, transmission function and conductance were obtained and discussed in the context of following problems.

- Phonon transport:
 - Bond reconstruction at contact surface:
 - Anharmonicity in nanostructure
 - Buffered layer between contact and nanostructure
 - Doping in nanostructure
 - Size effect of nanostructure
- Electron transport:
 - A discussion on thermoelectric efficiency
 - Electron scattering effect on thermoelectric efficiency