ENERGY CONVERSION PROCESSES BY FIRST PRINCIPLES
NONEQUILIBRIUM TRANSPORT CALCULATION

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Electric transport and energy conversion at nano-contact or interface systems are the most fundamental process for functional device such as nano-electronics, thermoelectricity, electrochemical catalysis, chemical cell, and nanofabrication. To understand these processes, detail mechanism of electric transport, phonon transport, local heating and current-induced force acting on ions should be clarified. Since they depend on detail structure of the junction and chemical species of contact, first principles calculation is highly desired.

Recent development of first principles calculation method based on nonequilibrium Green’s function (NEGF) theory allows us to estimated quantitative electric current at nano-contact and interface. To apply simulation to energy conversion processes, ion motions and interactions between electrons and ions have to be calculated by the same theoretical framework and accuracy with calculation of electric current.

In this talk, we will show our first principles results of the energy conversion processes at nano-contact including phonon transport and local heating effects. Though there are a few limitations in our theoretical model, we calculate explicitly phonon transport, electron-phonon interaction, and current-induced forces by first principles NEGF as well as electric transport. The first presentation is thermolectricity of organometallic molecular layers. Very recently, superior long range electric transport of organometallic wire (layer) has been reported by several groups. We will show analysis a potential of organometallic molecular material as thermoelectric device, and length dependence of ZT in the view of orbital engineering.

The second topic is control of molecular conformation by Scanning Tunneling Microscopy (STM), which is a promising technique of nanofabrication and molecular electronics. We perform a campaign of exhaustive first-principles calculations to obtain most of the parameters for current-induced reaction dynamics, and applied our theoretical model to the molecular conformation switching of melamine/ Cu(001) system. The detail mechanism of the action spectra will be discussed.

Figure. Promoting modes of the reaction by local heating (IETS calculation)