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Density functional theory, Molecular electronics, Quantum transport, Thermoelectricity & Memcomputing

We are “Computational physics Lab” (Figure 1) of the Electrophysucs Department, NCTU. We have developed many-body theory combined with density functional theory in scattering approaches to study current-induced effects in atomic/molecular junctions. Our primary research interests include the following three major parts: **(a) Molecular electronics:** we investigate I-V, local heating, shot noise, counting statistics, electron-vibration effects, current-induced force, etc (Figure 2). **(b) Themoelectricity:** We investigate the electric coefficient, electric conductance, and electric thermal conductance using the current-carrying wavefunction calculated from first-principles. We also investigate the phonon’s thermal conductance using the non-equilibrium molecular dynamic simulations. In addition to the exploration of possible device applications, such as thermoelectric nano-refrigerator and transistor powered by heat, the techniques also allow us to build up the phase diagram for ZT. (Figure 3). **(c) Memcomputing:** recently, there has been growing interest in a new computer prototype call “memcomputer”. These new, brain-inspired computing devices also could help to understand the workings of the human brain. We investigate the Ni-DNA biological system, shown as a multifunctional electronic component, which incorporates the functionality of memristor, memcapacitor, and redox enhance hysteresis effect. The redox state of Ni ions is controllable by external bias, making it possible to serve as a multi-state memory component for “memcomputer”.

Figure 1

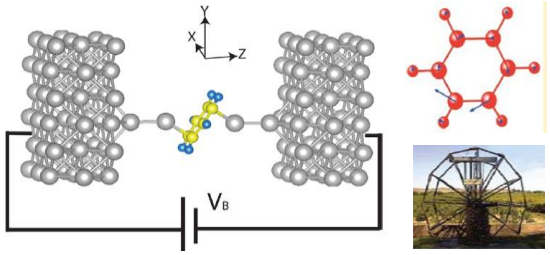

Figure 2: single-molecule motor driven by current-induced force

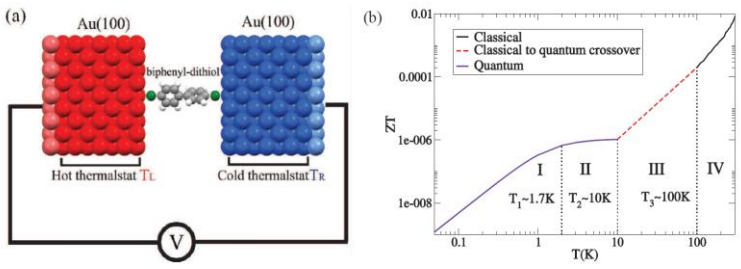

Figure 3 Phase diagram of ZT

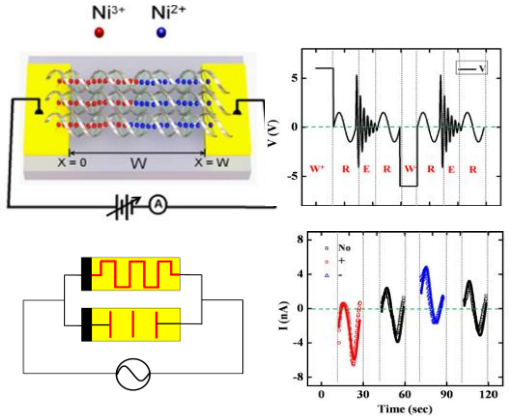

Figure 4 Ni-DNA as memristor, memcapacitor, and memory device.