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Thermoelectricity of C_{82} and $Gd@C_{82}$ Molecular Junctions

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There has been considerable interest in the studies on thermoelectricity of atomic and molecular junctions since it is proposed that the best thermoelectric efficiency can be achieved in charge transport through a single energy level [1]. Seebeck coefficient (S) of atomic and molecular junctions is described as a function of $d\tau/dE$, where τ and E represents transmission function and energy, respectively [1]. As the Fermi energy level (E_F) of the electrode is usually located between the transmission peak related to the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) level, the sign of S can indicate the energy level of the E_F relative to the HOMO or LUMO levels [2].

Recently, the endohedral metallofullerene (EMF) molecules have gained attraction due to their remarkable electrical and magnetic properties [3]. EMFs are expected to show larger S than empty C_{82} because they have lower ionization potentials and higher electron affinity than empty fullerenes [4], *i.e.*, molecular orbital level nearer to E_F .

In our experiment, the thermoelectric voltage of C_{82} and $Gd@C_{82}$ molecular junctions with Au electrodes was measured with a home build scanning tunneling microscope (STM). Temperature difference between the tip and the substrate was controlled by the substrate's temperature with a Peltier device. Si diode temperature

sensors were used to monitor the temperatures of the tip and substrate. The STM tip was brought close to the substrate until the threshold current value, that was larger than the current for a single molecular junction determined by break junction measurements, was reached. Then, the voltage difference between the tip and the substrate was measured during the retraction of the tip.

Figure 1 shows the thermoelectric voltage as a function of ΔT for Au- C_{82} -Au and Au- $Gd@C_{82}$ -Au, respectively. Negative S was observed for both C_{82} and $Gd@C_{82}$, which indicates the charge transport is through the LUMO level for both molecules. The S was found to be larger for Au- $Gd@C_{82}$ -Au junctions ($\sim 25\mu V/K$) compared to Au- C_{82} -Au junctions ($\sim 16\mu V/K$). The enhancement of the thermopower value shows the potential of EMF for high efficiency thermoelectric materials.

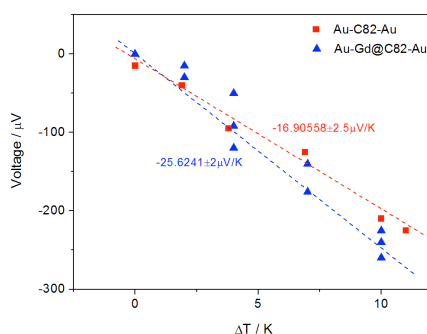


Figure 1: Thermoelectric voltage as a function of ΔT for C_{82} and $Gd@C_{82}$ molecular junctions.

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