Thermoelectricity in tunneling nanostructures

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We use the concept of resonant tunneling to calculate the thermopower of molecular nanosystems. It turns out that the sign of the thermovoltage under resonant tunneling conditions depends sensitively on the participating molecular orbital, and one finds a sign change when the transport channel switches from the highest occupied molecular orbital to the lowest unoccupied molecular orbital. Comparing our results to recent experimental data obtained for a BDT molecule contacted with an STM tip, we observe good agreement.

We study also a simple model to describe resonant tunneling through an organic molecule between to conducting leads, taking into account the vibrational modes of the molecule. We solve the model approximately analytically in the weak coupling limit and give explicit expressions for the thermopower and Seebeck coefficient. The behavior of these two quantities is studied as function of model parameters and temperature. For a certain regime of parameters a rather peculiar variation of the thermopower and Seebeck coefficient is observed.