Thermoelectricity at Molecular Length scale: A New Perspective

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ABSTRACT

The project deals with a thorough analysis of thermoelectric phenomenon in a magnetic helix possessing long range hopping (LRH) interactions. The magnetic helix is subjected to a circularly polarized light irradiation which plays the central role in our analysis. Simulating the quantum system within a Tight-binding framework, we evaluate all the thermoelectric quantities using Landauer prescription, and the two-terminal transmission probabilities are determined following the robust Green's function technique. The effect of irradiation is incorporated following Bloch-Floquet prescription using minimal coupling scheme through the hopping term. Quite interestingly we find that, electrical conductance as well as thermopower increases significantly at some typical Fermi energies whereas the thermal conductance due to electrons gets reduced at these energies, resulting a large figure of merit. The underlying physical mechanism of achieving large figure of merit (ZT ~ 4) relies on the asymmetric transmission function in such a LRH magnetic helix which is further enhanced in presence of light irradiation. In presence of the spin-dependent scattering, the up and down spin energy channels gets separated which leads to several interesting features in thermoelectric phenomena. Our analysis might be helpful in studying thermoelectric behaviour in different kinds of helical geometries and similar kind of fascinating systems having long range hopping interactions.

I. Introduction

To address the energy crisis across the globe conversion of waste heat into usable electrical energy has been considered as one of the major challenges both in science and technology over the past few [1].

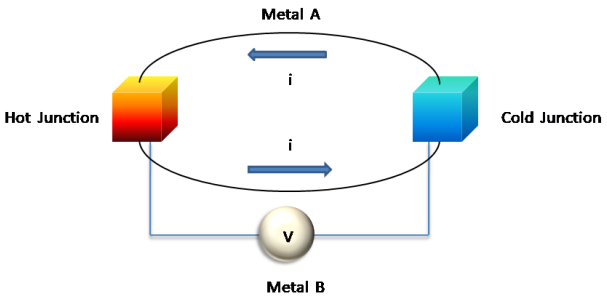

Figure 1: Schematic diagram of Seebeck effect where a thermal gradient induces a voltage drop at two junctions.

Out of many possible techniques, *Thermoelectric* (TE) energy conversion has been considered as one of the

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