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π-Stacked $(C_n\text{-}C_6H_6\text{–Fe–}C_6H_6\text{–}C_{13\text{-}n})_{n=2}$: A spin operated thermoelectric nanodevice

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ABSTRACT

Harvesting waste heat back into electricity by exploiting the temperature difference across two ends of a nanodevice and its concomitant spin dependence has led to the emergence of a new field known as spin caloritronics. Herein, we report the spin polarized thermoelectric features in a π-stacked system comprised of $(C_n\text{-}C_6H_6\text{–Fe–}C_6H_6\text{–}C_{13\text{-}n})_{n\,=\,2}$. A decisive factor, the Seebeck coefficient, becomes fully spin dependent on temperature and switches from positive to negative values, which illustrates the switching of the thermoelectric behavior from a p-to n-type due to the change in the spin state from spin-down to spin-up. A relatively large thermoelectric figure of merit has been reported in the case of the spin figure of merit of the system. In this context, three major observations have been made: i) The Seebeck coefficient has a distinctive feature over two different spin channels, ii) the spin Seebeck coefficient (S_s) is nearly four times larger than the charge Seebeck coefficient (S_c), and (iii) the spin thermoelectric figure of merit (Z_S) rises by 80% with respect to charge thermoelectric figure of merit (Z_C) under thermal bias. Our results have been well explained through the analysis of temperature dependent transmission spectra of the system. The emergence of a relatively large spin Seebeck coefficient allows us to measure the pure spin current of the system as well as extending the devices application from simple memory (MRAM) devices to on-chip energy harvesting systems.

1. Introduction

A clean and green energy solution to the loss of heat generated in our electronic and electrical appliances is to obtain electricity back from this thermal energy waste [1–4]. Over the years, physicists have been addressing this issue using simple and easily attainable devices known as thermoelectric materials, wherein the difference in temperature can produce electricity. Some of the notable, but powerful thermoelectric materials include $Mg_3(Sb,Bi)_2$, Cu_2Se, $CuInSe_2$ Bi_2Te_3, PbTe, SiGe, and Cu_2S [5–12]. However, most of these devices are bulk materials and not sufficient to address the waste heat developed in modern nanoelectronic devices. This issue has been highlighted in a number of recent studies along with demonstration of novel features, such as thermoelectric switching from p-type to n-type [13], in which the tunneling of electrons purely depends on the change in the thermal bias of the electrodes. In this efficient energy conversion technology, 2D nanostructures such as graphene have been proven to be highly effective. Modification in the thermoelectric features against the spin polarization of tunneling electrons has developed the new, but unexplored, domain of spincaloritronics. In this work we have focused on spin polarized thermoelectric features of a π-stacked system and its concomitant spin polarized thermoelectric switching behavior.

As reported in the literature, thermoelectric features are estimated using parameters such as the thermoelectric figure of merit (ZT), which is defined as follows: $ZT = G_\sigma S_\sigma^2 T/k$, where G_σ, S_σ, k, T are the spin polarized electrical conductivity, spin polarized Seebeck coefficient, thermal conductivity, and absolute temperature, respectively. The thermal conductivity contains contributions from both electrons and phonons. In spincaloritronics, one will have separate figure of merits for the charged and spin parts. The charge Seebeck coefficient is defined as follows: $S_C = \frac{G_\uparrow S_\uparrow + G_\downarrow S_\downarrow}{G_\uparrow + G_\downarrow}$ and the spin Seebeck coefficient is defined as

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