Thermoelectric Properties of Two-dimensional Dirac Materials in HgTe Quantum Wells

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Recent research focused on discovering new materials that exhibit superior performance and efficiency in the thermoelectric effect represents a leading trend in condensed matter physics. Prominent among these materials are novel semimetals, topological insulators, and Dirac materials. A critical factor enabling the exploitation of these materials' unique properties is the ability to manipulate their exotic electronic structures to boost thermoelectric efficiency.

The figure of merit for thermoelectric materials, denoted as ZT, is defined by the equation: $ZT = \frac{S_e^2 \sigma T}{\kappa}$ (1), where S_e represents the Seebeck coefficient, σ is the electrical conductivity, κ is the thermal conductivity, and T is the absolute temperature. Achieving high-performance thermoelectricity largely involves identifying materials that possess a significant Seebeck coefficient and elevated electrical conductivity or mobility.

The equation (1) together with Mott equation highlight that optimizing thermoelectric performance can be approached in two primary ways: enhancing the energy dependence of scattering mechanisms and employing band engineering strategies. These strategies involve leveraging a combination of highly dispersive bands and regular bands to enhance the electrical performance of thermoelectric materials. The first strategy involves leveraging 2D Dirac materials, where a significant enhancement in the thermoelectric coefficient has been expected, due to the unique transport characteristics of these materials. The second approach focuses on novel semimetals characterized by the simultaneous presence of highly dispersive (linear) and conventional regular (parabolic) bands. The k-linear bands are key to achieving high charge carrier mobility, contributing to improved electrical conductivity. On the other hand, the coexisting regular band, typically much denser than the dispersive topological bands, provides a substantial density of states (DOS) and enhances thermopower.

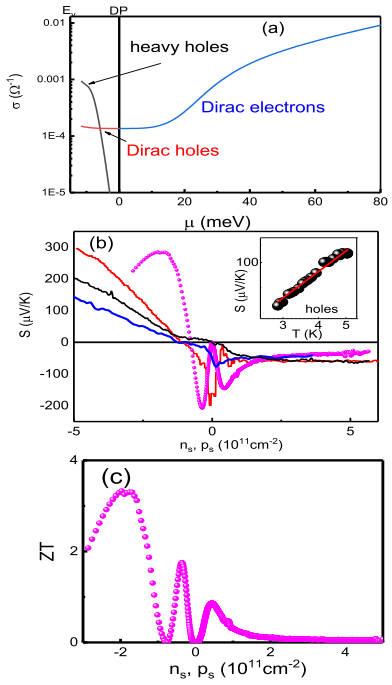

Fig. 1. (a) (a) Conductivity of the different subbands in gapless 6.3 nm HgTe quantum well as a function of the chemical potential (b) Seebek coefficient as a function of the density measured for different samples: Red line-sample A, blue line -sample B, black line -sample C, T=4.2 K. Insert- the temperature dependence of the Seebek coefficient for holes ($Vg = -4V$), solid red line $S \sim T^{1.5}$. Circles-theory calculated from the Mott equation. (c) Calculated figure of merit ZT as a function of the carrier density.

In our study, we introduce the HgTe quantum well as a comprehensive platform that aligns with both outlined strategies. There are several features that make the 2D Dirac semimetal in a gapless HgTe quantum well an attractive system for thermoelectricity studies. The single Dirac cone responsible for several important consequences can be derived from the Mott relation and can enhance the conductivity and Seebeck coefficient (figure 1a). In contrast to conventional 2D systems, the density of states varies with energy, and the transport time has a strong energy dependence. The coexistence of Dirac and heavy holes creates an unusual situation for manipulating the band degeneracy. In this study, we have measured the Seebeck coefficient in a 6.3 nm HgTe well and demonstrated that some of these possibilities can be developed in this system. The behavior of the Seebeck coefficient is explained based on the Mott relation (figure 1b,c).