# Valley-dependent electron-phonon scattering in thermoelectric semimetal $Ta_2PdSe_6$

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High-performance thermoelectric materials have long been sought mainly among lightly doped insulators and semiconductors. This is because electrons and holes contribute with opposite signs to the Seebeck effect, so metallic systems typically exhibit a small Seebeck coefficient. Recently, however, it has attracted considerable attention that electron-hole asymmetry in relaxation time can yield a high thermoelectric power factor even in metals.

The quasi-one-dimensional transition-metal chalcogenide $Ta_2PdSe_6$ is a promising thermoelectric semimetal that shows high thermoelectric performance at low temperatures [1,2]. Experiments have shown that the mobilities of electron and hole carriers differ by an order of magnitude at low temperature. Although some studies have investigated its electronic band structure and the phonon band dispersion, the scattering properties of carriers have not yet been theoretically examined

In this study [3], we perform first-principles calculations of electron-phonon scattering in $Ta_2PdSe_6$ using Quantum ESPRESSO and EPW [4]. We find that the imaginary part of the electron self-energy, Im Σ, is roughly proportional to the electronic density of states (shown as a red line) but exhibits a pronounced peak near the Fermi level [see Fig. 1]. As shown in Fig. 2, the electron self-energy is strongly *k*-dependent and strong intervalley scattering occurs between the electron pocket and the highest valence band at the Γ point. This strong scattering is associated with a soft phonon mode. We also discuss the possible enhancement of the Seebeck coefficient due to this strongly energy-dependent scattering rate. Our study clarifies intriguing valley-dependent electron-phonon scattering in $Ta_2PdSe_6$.

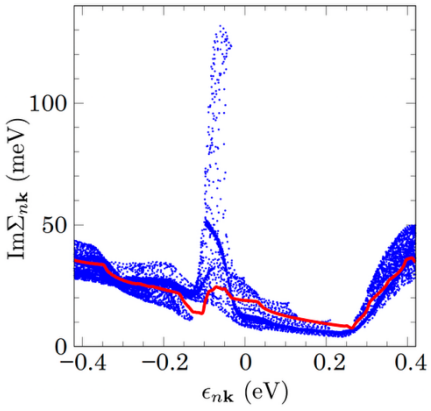


Figure 1: Imaginary part of the electron self-energy, Im Σ.

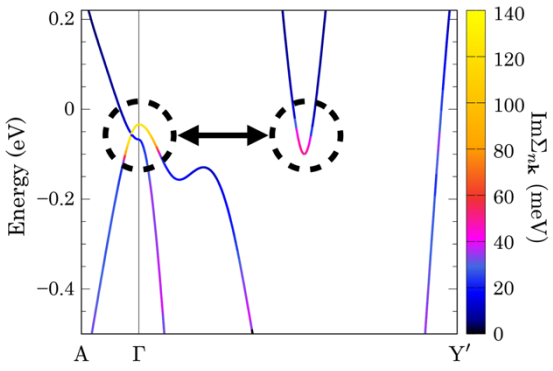


Figure 2: Im Σ shown on the electronic band structure.

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