Supporting information II

Theoretical Study of Lifshitz Transition for 2H-TaS_2

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The calculations of transport properties are based on the semi-empirical Boltzmann transport theory. The group velocity of electron can be expressed as follows:

$$v_\alpha(i,k) = \frac{1}{\hbar}\frac{\partial \varepsilon_{i,k}}{\partial k_\alpha}$$

where, $\varepsilon_{i,k}$ is the energy eigenvalue for the ith energy band at the k point. α denotes the velocity along the α direction. The conductivity tensor can be expressed as follows:

$$\sigma_{\alpha\beta}(i,k) = e^2 \tau_{i,k} v_\alpha(i,k) v_\beta(i,k)$$

In the above equation, $\tau_{i,k}$ is the relaxation time. $v_a(i,k)$ and $v_\beta(i,k)$ are the group velocities, i.e., the drift velocities. In general, the relaxation time $\tau_{i,k}$ is related to both the ith band and the direction of k vector. Under the constant relaxation time approximation, $\tau_{i,k}$ can be regarded as a constant independent of the carrier energy. Although the constant relaxation time approximation has limitations, this approximation simplifies the transport mechanism of carriers inside the material. In the case where the energy and temperature dependence of carrier scattering is small, all the relaxation times in the system will be very close to their average values, and then the transport coefficients at the constant relaxation time approximation are more reliable in this case. The doping concentration, i.e. the carrier concentration, determines the Fermi energy level. In general, in the lower doping concentration, the number and type of doping on the energy band structure of the system in the vicinity of the energy gap can be ignored, at this time only the Fermi energy level will move with the change of doping concentration, which is known as the rigid energy band model. The conductivity under the rigid energy band model approximation is related to the transport distribution function, with

$$\sigma_{\alpha\beta}(\varepsilon) = \frac{1}{N}\sum_{i,k}\sigma_{\alpha\beta}(i,k)\frac{\delta(\varepsilon - \varepsilon_{i,k})}{\mathrm{d}\varepsilon}$$

where N is the number of k points in the calculation. It is clear that the transport coefficient is a function of the chemical potential μ (Fermi energy) and the temperature T . After integrating the transport distribution function over the whole space, the following transport parameters of the semiconductor can be obtained. The conductivity can be expressed as

$$\sigma_{\alpha\beta}(T;\mu) = \frac{1}{\Omega}\int \sigma_{\alpha\beta}(\varepsilon)\left[-\frac{\partial f_\mu(T;\varepsilon)}{\partial \varepsilon}\right]\mathrm{d}\varepsilon$$

where, $f(T;\varepsilon)$ is the Fermi-Dirac distribution function. In the calculation of conductivity, the intrinsic energy $\varepsilon_{i,k}$ at point k needs to be found, and $\varepsilon_{i,k}$ can be obtained from the energy band structure of the material. The carrier concentration can be found by varying the chemical potential μ with respect to the different positions of the energy bands.