Anomalous Thermoelectric Transport in biased bilayer WSe_2

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Two-dimensional (2D) materials with hexagonal structure and transition metal dichalcogenides (TMDs) are furnished with inequivalent valleys at the K and K' points of the Brillouin zone, which are local extrema of the electronic band structure [1]. In these materials an electron not only has spin, but also a valley degree of freedom, which acts as a pseudospin. Promising possibilities for spintronic and valleytronic devices for logic and memory with ultra-low power dissipation have been proposed. However, research in understanding phenomena such as valley- and spin-Hall effects for the K and $K' = -K$ Dirac valleys is still at the fundamental level [1]. The realization of these effects is based on the control of properties that differ between the two valleys [2] in particular the Berry curvature ($\mathbf{\Omega}$) upon braking of space-inversion (*P*) symmetry. The Berry curvature gives rise to the valley-Hall effect in which electrons at the two valleys drift to opposite edges of the material in the presence of an in-plane electric field due to the equal but opposite Berry curvatures at the two valleys (see Fig. 1). A nonzero $\mathbf{\Omega}$ in TMDs also leads to various anomalous transport phenomena. In this work, we investigate the berry curvature and one of these effects, the anomalous Nernst effect (ANE) [3] in bilayer WSe_2 with broken *P* symmetry via gating.

In Fig. 2 we show the energy dispersion $E^{\mu}_{\lambda s_z}$ of bilayer WSe_2 for the K valley versus k/k_c where $k_c = \pi/a$ and $a = 3.32$Å is the lattice constant, $\lambda = c(v)$ for the conduction (valence) band, $\mu = +1(-1)$ is the layer pseudospin for the top (bottom) layer, and s_z is the spin. For finite electrostatic energy V, the spin degeneracy of the subbands is lifted. In bilayer TMDs, for $V = 0$ the origin of finite $\mathbf{\Omega}(\mathbf{k})$ is the SOC as shown in Fig. 3. In Fig. 4 notice that for $V \approx 7.5$meV, which is the SOC for electrons, $\Omega^b_{c,\downarrow} = \Omega^t_{c,\downarrow}$. Also, $\Omega^b_{v,\downarrow} = \Omega^t_{v,\downarrow}$ at $V \approx 112.5$meV, which is the SOC for holes. The ANC is shown in Fig. 5 for increasing values of V. For $V = 0$, P is preserved and $\alpha^v_{xy} = 0$. However, a $V > 0$, leads to finite α^v_{xy}, whose magnitude and sign is proportional the $\mathbf{\Omega}(\boldsymbol{k})$ of the respective bands, and can be controlled by *V*. In a similar manner, in Fig. 6 the spin-Nernst effect is also controlled by *V*.

[1] D. Xiao et al., Phys. Rev. Lett. **108**, 196802 (2012); [2] D. Xiao et al., Phys. Rev. Lett. **99**, 236809 (2007); [3] V. Vargiamidis et al., Phys. Rev. B **102**, 235426 (2020).

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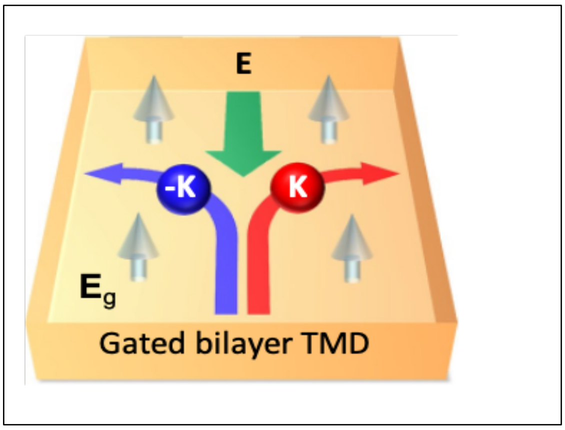

Fig.1: Valley Hall effect in bilayer transition metal dichalcogenide (TMD) in the presence of in-plane and out of plane electric fields ***E****, and* $\boldsymbol{E}_g$*, respectively (*$\boldsymbol{E}_g$*, shown by the out-of-plane white arrows).*

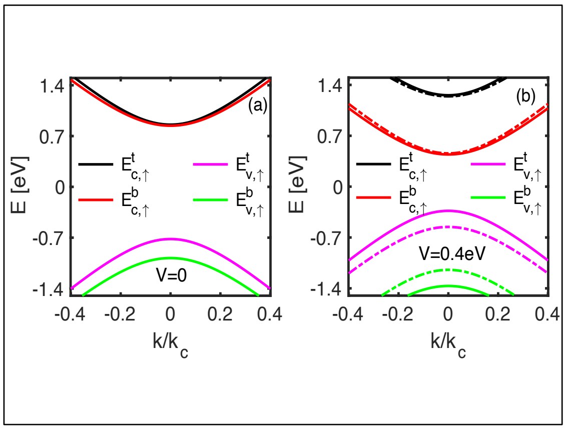

Fig.2: Energy dispersion near the ***K*** *valley for bilayer WSe2 in the absence (left panel) and presence (right panel) of a perpendicular electric field corresponding to a potential energy $V = 0.4$eV. The solid curves are for spin-up bands and the dash-dotted ones for spin-down.*

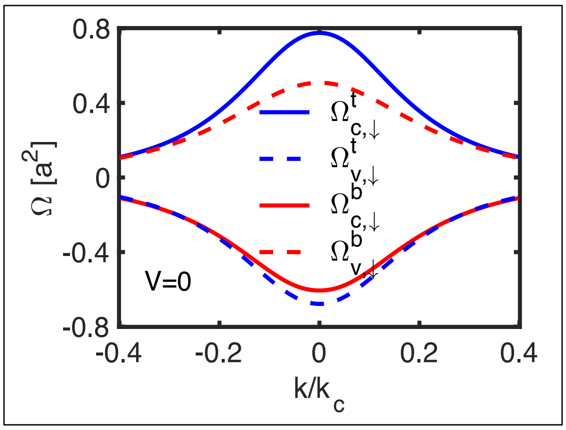

Fig.3: Berry curvature $\Omega(\boldsymbol{k})$ of spin-down bands versus k/k_c near the ***K*** *valley for zero electrostatic potential (V=0). Distributions of $\Omega(\boldsymbol{k})$ have opposite signs in the* ***K'***=−***K*** *valley.*

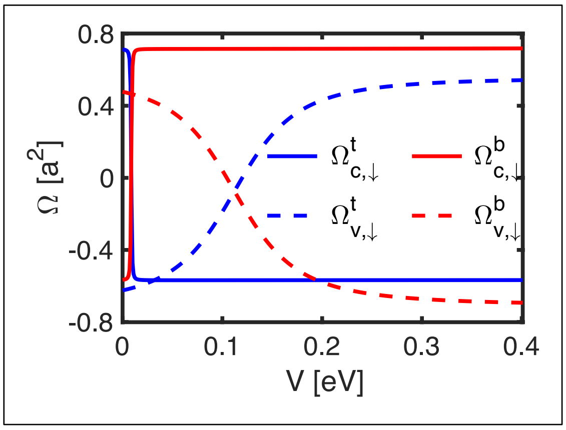

Fig.4: Berry curvature of spin-down bands versus V for $k/k_c \simeq 0$. The polarity of $\Omega(\boldsymbol{k})$ changes when V=7.5meV or 112.5meV, i.e., at the values of spin-orbit coupling for electrons and holes.

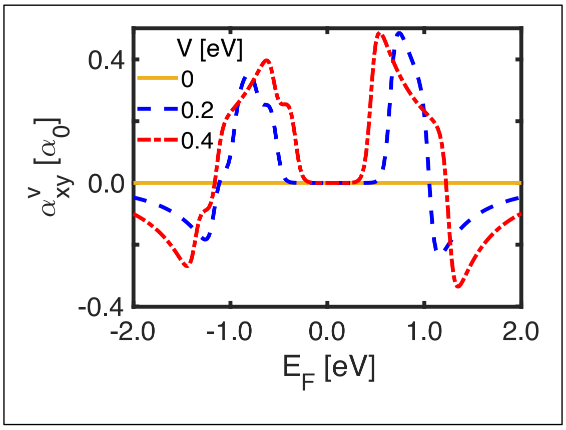

Fig.5: Anomalous Nernst coefficient (ANC) α^v_{xy} for the ***K*** *valley versus E_F for increasing values of electrostatic potential V, in units $\alpha_0 = ek_B/4\pi^2\hbar$. The temperature is T=300*K.

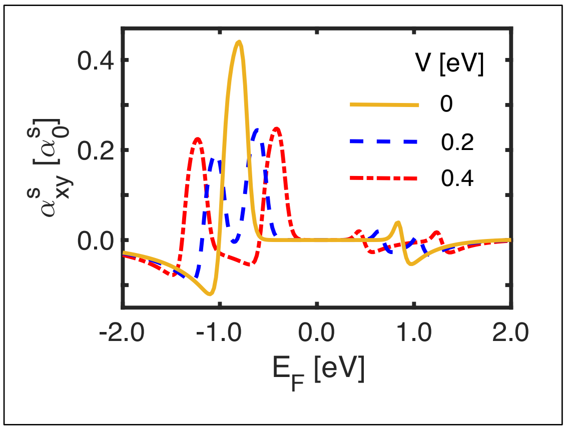

Fig.6: Spin Nernst coefficient (SNC) α^s_{xy} for the ***K*** *valley versus E_F for increasing values of electrostatic potential V, in units $\alpha_0^s = \alpha_0(\hbar/2e)$. The temperature is T=300*K.