Comment on "HgSe: Metal or Semiconductor?"

In a recent Letter Gawlik *et al.* [1] interpret their angle resolved photoemission (PE) and angle resolved inverse PE from HgSe as pointing to an open gap configuration of the Γ_6 and Γ_8 bands. This contradicts the commonly accepted picture based on transport [2] and even more direct optical and magnetooptical [3] data which demonstrated an occurrence of the inverted band structure similar to that of HgTe. The latter was also consistent with the investigations of alloys of HgSe involving Cd, Zn, and Fe [4] as well as Mn [5]. Here, we show that the amazingly accurate data of Gawlik *et al.* [1] can be understood without invoking the open gap configuration in the bulk material.

As it is well known, at a surface of any semiconductor there usually exist surface charges resulting in an electric field, i.e., band bending, perpendicular to the surface. This may lead to formation of an electron accumulation layer as it does take place in, e.g., InAs [6] or $Hg_{1-x}Cd_xTe$ [7]. The electric field near the surface and the corresponding one-dimensional potential well lowers the cubic symmetry of HgSe and lifts the fourfold degeneracy of the Γ_8 band. More specifically, the role of such a potential well is twofold. First, it leads to formation of two-dimensional electron states at the surface [8]. Second, it repulses out of the surface those heavy-hole states which reside above the bottom of the potential well. Thus, they cease to contribute to PE, as the escape length of the photoelectrons is shorter than the distance of these states from the surface. As a result a gap appears in the PE spectrum.

The question is whether a realistic surface charge density can produce the splitting between the edges of the density-of-states at the surface that would be in agreement with the observations [1]. Neglecting tunneling between the bands one can construct a simple theory of energy levels confined in an accumulation layer due to a linear surface electric field, with the field strength being the parameter of the theory [9]. Such a theory can be formulated including nonparabolicity effects and, thus, possess a quantitative character. Assuming that the energy separation of $\sim$400 meV observed in [1] (and interpreted as the evidence of the configuration with the Γ_6 band above Γ_8) corresponds to the energy position of the ground electric subband in the triangular potential well in respect to its bottom one can estimate the field $\mathcal{E}$ that leads to the above value: with the accepted masses of electrons in HgSe at room temperature one obtains $\mathcal{E} = 7 \times 10^5$ V/cm. Then the energy of the bottom of the ground and excited electric subband is $E_1 = 397$ meV and $E_2 = 625$ meV, respectively. We note that the width of the potential well at E_1, $E_1/e\mathcal{E} = 57$ Å is consistent with the Thomas-Fermi screening length for HgSe where typical electron concentration is 2×10^{18} cm^{-3} [2], i.e., $\lambda_{TF} = 65$ Å. Since there are at least two states discernible in the region of interest in Fig. 1 of Ref. [1] one has to assume that these two electric subbands are occupied by electrons in the sample studied by these authors. This corresponds to the energy of the surface impurity state that pins the Fermi level to be roughly $E_S = 0.65$ eV above the Γ_8 point. Because of the highest electron affinity among II-VI compounds [10], the value of E_S can, in fact, be particularly large in HgSe.

Thus, we would like to associate the asymmetric peak in Fig. 1 of Ref. [1] (resembling a doublet structure) with the presence of two occupied electric subbands, exactly like in the case of recently studied PE in InAs [11]. In the photoemission spectra, these states are separated from the valence band continuum of states since the latter are repulsed from the surface by the electric field produced by the electron accumulation layer.

In view of these facts our feeling is that the experiments of Gawlik *et al.* are not in contradiction with the inverted band arrangement of bulk HgSe.

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