Erratum: Spin Chirality Tuning and Topological Semimetals in Strained $\text{HgTe}_x\text{S}_{1-x}$ [Phys. Rev. Lett. 114, 236805 (2015)]

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As discussed in the Letter, the unusual ordering of the p bands in HgS originates from the spin-orbit coupling (SOC) of the d bands which influence the p bands via pronounced p - d hybridization. In our tight-binding (TB) model, this has been described effectively by a negative SOC parameter λ_p of the p bands while keeping a zero SOC parameter λ_d of the d bands. This approximation reproduces the ordering of the p bands; however, minute effects that originate from the bulk-inversion asymmetry of the zinc blende structure are neglected.

To account for the bulk-inversion asymmetry we improved the TB parameter sets of both HgTe and HgS by including explicitly the SOC parameters λ_d of the d bands (Table I) and recalculated the topological phase diagram (Fig. 1). Instead of a topological Dirac semimetal phase (DSM), we find another Weyl semimetal phase, called WSM II; all other topological phases are preserved. The phase boundaries are insignificantly shifted due to the improved TB parameter set.

To explore the WSM II phase in more detail we focus on the bulk band structure for tensile strained HgTe ($x = 1.0$, $\beta = 0.97$), calculated by both our *ab initio* KKR and TB methods. In both calculations, two tiny gaps of about 2 meV open

FIG. 1. Topological phase diagram of strained $\text{HgTe}_x\text{S}_{1-x}$ alloys (x alloy concentration, β strain). The phases are indicated by colors: strong topological insulator (STI) with mirror Chern number $c_m = -1$ (red), STI with $c_m = +1$ (green), Weyl semimetal (WSM I & WSM II, grey), and normal semimetal (blue).

FIG. 2. Weyl semimetal phase WSM II in tensile strained HgTe ($\beta = 0.97$). (a) *Ab initio* KKR band structure along the $-Z - \Gamma - Z$ line showing a band gap between the topmost valence and lowest conduction bands. (b) Width E_g of the band gap in the $k_x k_y$ plane with $k_z = +56 \text{ m}^{-1}$, indicated as color scale (black: $E_g > 7 \text{ meV}$, white: $E_g = 0 \text{ meV}$; TB calculation). Four Weyl points are marked by green dots.

TABLE I. Slater-Koster tight-binding parameters for HgTe and HgS (in eV). Only data that differ from the original set are given. The spin-orbit coupling strength λ_p is for Te and S, whereas all other parameters are for Hg interactions.

	λ_p	λ_d	$(dd\sigma)$	$(dd\pi)$	$(dd\delta)$
HgTe	0.31	0.33	-0.094	0.05	0.03
HgS	-0.02	0.32	...	...	...

up along the $-Z - \Gamma - Z$ line [Fig. 2(a)]. Each band gap opening is accompanied by the presence of four Weyl points [Fig. 2(b)]. Put differently, the two Dirac points in the DSM phase which showed up for $\lambda_d = 0$ split up into eight (2×4) Weyl points for $\lambda_d \neq 0$. These Weyl points are located very close to the $-Z - \Gamma - Z$ line, namely at $(\pm\tilde{k}_{\parallel}, 0, \pm\tilde{k}_z)$ and $(0, \pm\tilde{k}_{\parallel}, \pm\tilde{k}_z)$, with $\tilde{k}_{\parallel} = 0.36 \text{ m\AA}^{-1}$ and $\tilde{k}_z = 56 \text{ m\AA}^{-1}$. These findings confirm those reported in Ref. [1]; however, $\tilde{k}_{\parallel}$ is one order of magnitude less than its analogue in that publication, which we attribute to details in the *ab initio* computations and in the TB parametrization, as well as to the modeling of strain.

To sum up, accounting for the bulk-inversion asymmetry in the d bands leads to a Weyl semimetal phase (WSM II) in tensile strained HgTe, in contrast to the topological Dirac semimetal (DSM) phase reported in the Letter. The eight Weyl points are so close to the $-Z - \Gamma - Z$ line of the bulk Brillouin zone that it may be difficult to distinguish the WSM II from the DSM phase in experiments.

[1] J. Ruan, S.-K. Jian, H. Yao, H. Zhang, S.-C. Zhang, and D. Xing, *Nat. Commun.* **7**, 11136 (2016).