ERRATA

Erratum: Occupied and unoccupied electronic band structure of WSe_2 [Phys. Rev. B 55, 10 400 (1997)]

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The band-structure calculation for $2H$-WSe_2 presented in Refs. 1 and 2 was based on an erroneous value of the c-axis lattice parameter (13.459 Å instead of 12.960 Å), which resulted from a mistyping during conversion into atomic units. The a-axis constant was not affected. The corrected band structure is shown in Fig. 1, together with the original spectroscopic data of Ref. 1. Total energy optimization yields a W-to-Se layer separation $z \times c$ with $z_{\mathrm{theo}} = 0.1307$ (before: 0.126) that is now in better agreement with the experimental value of $z_{\mathrm{exp}} = 0.129$. The smaller c-axis constant increases the ΓA bandwidth of the topmost W $5d_{z^2}$/Se $4p_z$-like valence band by about 20%. As a consequence and contrary to the original result, the calculation now places the valence-band maximum (VBM) at the Γ point, lying 98 meV (41 meV) above the highest occupied state at K when using the experimental (theoretical) structure parameter z. This result brings our calculation into qualitative agreement with other theoretical work, but is now at variance with the photoemission data in Ref. 1 that locates the VBM at the K point. Band calculations for a finite number of Se-W-Se slabs give evidence that surface effects on the electronic structure may be responsible for the discrepancy between photoemission and bulk band theory. Details will be presented elsewhere.

Other conclusions of Refs. 1 and 2 concerning the orbital character of the bands, the strong W 5d-Se 4p covalency, and the importance of spin-orbit coupling are not affected. Apart from the question on VBM position, there is still good overall (in parts even better) agreement between theory and experiment, as can be seen in Fig. 1.

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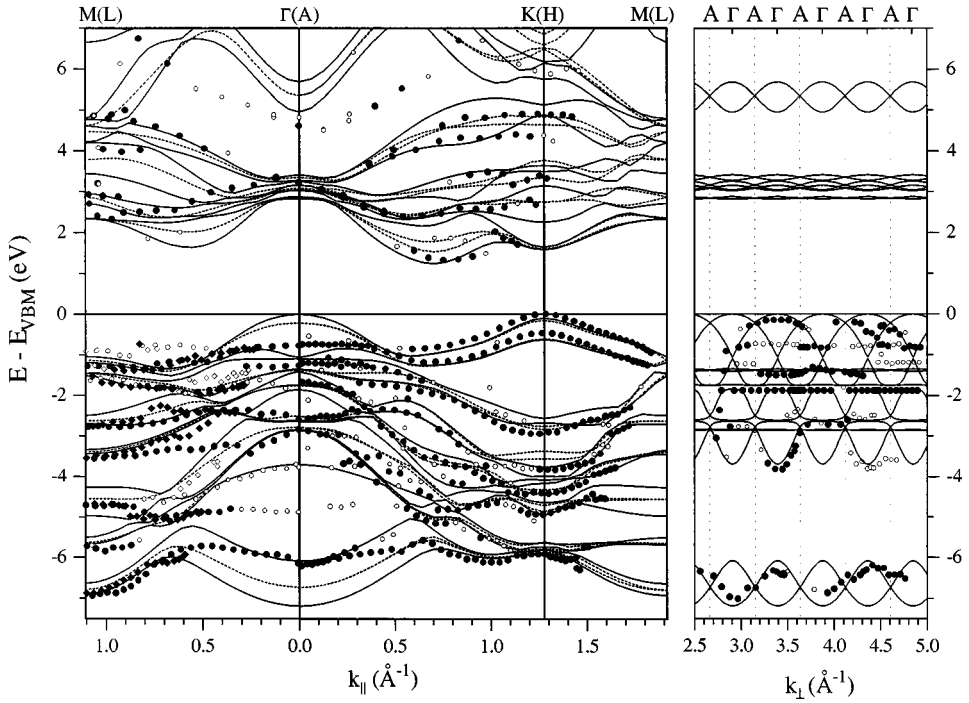

FIG. 1. Corrected band-structure calculation for $2H$-WSe_2 ($z = z_{\mathrm{exp}}$) in comparison to photoemission and inverse photoemission data (experimental data identical to Ref. 1). Solid and dashed lines in the left panel correspond to bands in the ΓKM and AHL planes, respectively. The separation between occupied and empty bands has been adjusted to match the measured direct optical gap of 1.7 eV at the K point. Solid (open) symbols denote strong (weak) experimental structures; diamonds are data points obtained by backfolding into the first Brillouin zone.

[1] Th. Finteis, M. Hengsberger, Th. Straub, K. Fauth, R. Claessen, P. Auer, P. Steiner, S. Hüfner, P. Blaha, M. Vögt, M. Lux-Steiner, and E. Bucher, Phys. Rev. B **55**, 10 400 (1997).

[2] Th. Straub, K. Frauth, Th. Finteis, M. Hengsberger, R. Claessen, P. Steiner, S. Hüfner, and P. Blaha, Phys. Rev. B **53**, R16 152 (1996).

