Abstract Submitted
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Non-topological 2DEG at the surface of YbB_6 and Divalent Hexaborides[1] J.D. DENLINGER, Lawrence Berkeley Nat'l Lab, C.H. MIN, F. REINERT, U. Wuerzburg, BOYOUN KANG, GIST, D.J. KIM, Z. FISK, UC Irvine, K. GOTLIEB, A. LANZARA, UC Berkeley, C.-J. KANG, B.I. MIN, POSTECH, J.W. ALLEN, U. of Michigan — A recent theoretical prediction of YbB_6 being an f-d band-inverted mixed-valent topological insulator very similar to SmB_6 [1] and subsequent angle-resolved photoemission topological interpretations of V-shaped electron pockets [2] are at odds with the previous experimental classification of the material as a divalent small p-d band gap semiconductor. Our angle-resolved photoemission of the (001) surface of YbB_6 confirms the nearly pure divalency of Yb and demonstrates that in-gap surface electron pockets, with slightly non-parabolic dispersion indicative of a small p-d gap, originate from quantum well states confined to the inversion layer of n-type surface regions with cation termination. Spatial- and time-dependent variations of the surface Fermi-level pinning are shown to be universal polar-surface-driven features of the semiconducting divalent hexaborides including CaB_6, SrB_6 and EuB_6 Also DFT+U+SO+mBJ theoretical band calculations are able to reproduce the experimental energy ordering of a p-d gap existing at E_F above the Yb 4f states with no f-d or p-d band inversions.

[1] H. Weng, et al., PRL 112, 16403 (2014).
[2] M. Xia, et al. arXiv:1404.6217; M. Neupane, et al., arXiv:1404.6814; N. Xu, et al., arXiv:1405.0165.

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