# Ab initio electronic structure, Fermi surface, and band topology of the correlated superconductor $YbBi_2$

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We present a first-principles study of the layered bismuthide $YbBi_2$ , a quasi-two-dimensional compound recently established as a type-I superconductor hosting topologically nontrivial states. Using two complementary density-functional-theory frameworks - the all-electron APW+lo method (WIEN2k) and the PAW pseudopotential approach (VASP) - with the GGA+U scheme and spin–orbit coupling, we describe the strongly correlated Yb 4f shell. The Hubbard parameter (U = 5.65 eV in WIEN2k, 6.35 eV in VASP) was fixed by matching the calculated density of states to angle-integrated photoemission, reproducing the $4f_{5/2}$ and $4f_{7/2}$ flat bands and the $\approx$1.3 eV spin–orbit splitting. Both methods yield a consistent electronic structure, a bulk Van Hove singularity near Γ, and a symmetry-protected fourfold band degeneracy along Z–T. From the Fermi surface, we obtain de Haas–van Alphen frequencies and effective masses. Surface bands for the (010) cleavage plane, evaluated with an in-house projector code, agree with ARPES maps. A Wannier90-based analysis of the Berry curvature around the T–Z line, using adaptive mesh refinement, gives a Berry phase $\varphi_B \approx 0.84\pi$, in close agreement with the value $\approx 0.82\pi$ extracted from the quantum-oscillation Landau-fan analysis. These results indicate the onset of nontrivial band topology and establish $YbBi_2$ as a platform for topology, correlations, and superconductivity in f-electron systems.

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