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Type-II Dirac cones as unified topological origin of the exotic electronic properties of WTe_2[1] LUKAS MUECHLER, Dept. of Chemistry, Princeton University, ARIS ALEXANDRADINATA, Dept. of Physics, Yale University, TITUS NEUPERT, Princeton Center for Theoretical Science, ROBERTO CAR, Dept. of Chemistry, Princeton University — WTe_2 is a recently discovered layered material with remarkable electronic properties. Transport measurements show an extremely large non-saturating magnetoresistance (MR) with mobilities as high as 167 000 cm^2/Vs at 2 K. Furthermore, recent photoemission experiments discovered circular dichroism in the bulk band structure. We propose a unified explanation for these exotic observations by relating key properties of the bulk electronic structure to that of to that of the mono- and bi-layer material. In particular, we demonstrate that the monolayer is a novel type-II Dirac semimetal in absence of spin-orbit coupling, with Dirac cones that are sufficiently anisotropic to simultaneously harbor electron and hole pockets. The band structure can be characterized by a new $Z_2 \times Z_2$ topological invariant defined through non-Abelian Wilson loops. We develop a tight-binding model for the mono- and bilayer of WTe_2 based on Wannier functions from *ab-inito* calculations and extend our findings to the iso-structural compounds $MoTe_2$ and ZrI_2.

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