## Detection of Dirac/Weyl Fermions via electron-states resolved NMR crystallography.

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The interest in the role of topology in condensed matter physics has been significantly increased over the last decade, with topological insulators and Dirac/Weyl semimetals being the most relevant systems featuring non-trivial topology. The state-of-the-art method to detect topological electron energy bands is Angle Resolved Photoemission Spectroscopy. However, despite its great effectiveness, there is a particular shortage in monitoring and manipulating Dirac and Weyl fermions, which appear as low energy quasiparticle excitations.

Herein, we show that by applying DFT-assisted broadband high-resolution solid-state Nuclear Magnetic Resonance (NMR) methods on microcrystalline WTe<sub>2</sub> [1] (type-II Weyl semimetal) and Bi<sub>2</sub>Te<sub>3</sub> nanoplatelets [2] (topological insulator), it is possible to routinely resolve complex ssNMR patterns into individual NMR resonances and precisely tie those resonances to the Dirac/Weyl electron states via their electron-nuclear hyperfine coupling. Electron-states resolved NMR crystallography is thus enabling the detection of Dirac and Weyl Fermions. References

[1] W. Papawassiliou et al., Phys. Rev. Research 4, 033133 (2022).

[2] W. Papawassiliou et al., Nat Commun **11**, 1285 (2020).



## **Figure 1:** Experimental (a) and DFT calculated (b) <sup>125</sup>Te aMAT NMR spectra of microcrystalline WTe<sub>2</sub>. (c-f) The k-resolved p-DOS of the p-orbitals (c,d) and s-orbitals (e,f) for each of the inequivalent sites present in the crystal structure. The large anisotropy of the NMR shift of Te(1,3) is driven by the p-orbital character of these sites, while the occupied s-orbitals of Te(2,4) are responsible for the observed positive shift in the NMR spectrum with respect to the Te(1,3) resonance [1].

## Figures