Importance of nonlocal electron correlation in the $BaNiS_2$ semimetal from quantum oscillations studies

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Quasi 2D $BaNiS_2$ exhibits an anomalously large spin-orbit Rashba coupling, even in the absence of heavy (electronically active) element ($Z_{Ni} = 28$) [1]. The magnitude of the splitting, which is due to the presence of a staggered electric field at the Ni site in a pyramidal environment, is comparable to the highest measured values [2]. This makes $BaNiS_2$ a candidate for applications involving the transport of spins rather than charges.

By a combined study of Shubnikov de Haas and de Haas van Alphen effects on high-quality single crystals, the Fermi surface of $BaNiS_2$ is investigated. Quantum oscillations show the occurrence of three extremal orbits. Ab initio electronic structure calculations, in the DFT framework, show that the inclusion of screened exchange, through a HSE hybrid functional with 7% of exact exchange, is necessary to account for the experimental Fermi pockets. The importance of non-local screened-exchange interactions in $BaNiS_2$, and, more generally, in 3*d* compensated semimetals, is underlined [3].

[1] D. Santos-Cottin et al., Nature Commun. **7**, 11258 (2016)
[2] H.M. Benia et al., Phys. Rev. B **94**, 121407(R) (2016)
[3] Y. Klein et al., Phys. Rev. B **97**, 075140 (2018)

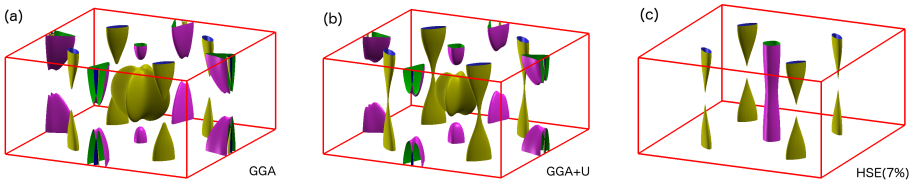

Figure 1: Fermi surfaces of $BaNiS_2$ from ab initio calculations with GGA (a), GGA + U (= 3 eV) (b), and modified HSE with 7% of exact exchange (c).