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BaNiS_2 monolayer as possible Z2 topological insulator

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After having been considered as a potential candidate for high-temperature superconductivity, the BaNi_xCo_{1-x}S_2 compound has seen a renewed attention for its fascinating spin properties, discovered only very recently [1,2]. BaNiS_2 is a Dirac semimetal, with 4 Dirac cones lying at the Fermi level. The cones, made of d-orbitals, are massive due to a large spin-orbit coupling, leading to a remarkable Rashba splitting of up to 0.15 eV. The spin-orbit coupling strength is unexpected, because BaNiS_2 is centrosymmetric and does not contain heavy elements. This places the compound very close to a topological insulating phase. By ab initio calculations, we give evidence of the possible realization of a robust Z2 topological phase in the BaNiS_2 monolayer.

[1] David Santos-Cottin, Michele Casula, Gabriel Lantz, Yannick Klein, Luca Petaccia, Patrick Le Févre, François Bertran, Evangelos Papalazarou, Marino Marsi, and Andrea Gauzzi. Rashba coupling amplification by a staggered crystal field, Nature Communications 7, 11258 (2016).
[2] Yannick Klein, Michele Casula, David Santos-Cottin, Alain Audouard, David Vignolles, Gwendal Fève, Vincent Freulon, Bernard Plaçais, Marine Verseils, Hancheng Yang, Lorenzo Paulatto, and Andrea Gauzzi, Importance of nonlocal electron correlation in the BaNiS_2 semimetal from quantum oscillations studies, Physical Review B 97, 075140 (2018).

Choix de session parallèle

3.3 Propriétés remarquables des matériaux topologiques : de la théorie à la réalisation expérimentale

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