Ab initio relativistic k·p models for non-centrosymmetric systems with competing spin-orbit and magnetic exchange interaction

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In this contribution, we present a fully *ab initio* relativistic **k·p** perturbation approach to *microscopically* generate effective Hamiltonians of a desired size [1, 2]. The approach allows one to make an effective **k·p** model capable of correctly reproducing the observable (true) spin polarization of two-dimensional (2D) states split by spin-orbit interaction (SOI) in non-centrosymmetric systems. In turn, this enables a proper treatment of the effect of magnetic exchange interaction of 2D-state electrons with a ferromagnetic substrate or supporting layer. As an example of the efficiency of our approach, in Figure 1 we show the specific SOI-induced spin polarization of the Si-terminated surface states of the rare earth (*R*) intermetallic compounds RT_2Si_2 (*T*=Ir, Rh) [2], which is characterized by a triple winding of surface-electron spins around the Fermi contours (FCs). The resulting complex spin structure underlies the shape of the FCs in the presence of the magnetic order in the rare-earth layers of RT_2Si_2. Applications of the approach to topological insulators, surface alloys, and structural elements of layered polar semiconductors are also presented in this contribution.

References

[1] I. A. Nechaev and E. E. Krasovskii, *Relativistic **k·p** Hamiltonians for centrosymmetric topological insulators from ab initio wave functions*, Phys. Rev. B **94**, 201410(R) (2016).
[2] I. A. Nechaev and E. E. Krasovskii, *Relativistic splitting of surface states at Si-terminated surfaces of the layered intermetallic compounds RT_2Si_2 (R=rare earth; T=Ir, Rh),* Phys. Rev. B **98**, 245415 (2018).

Figures

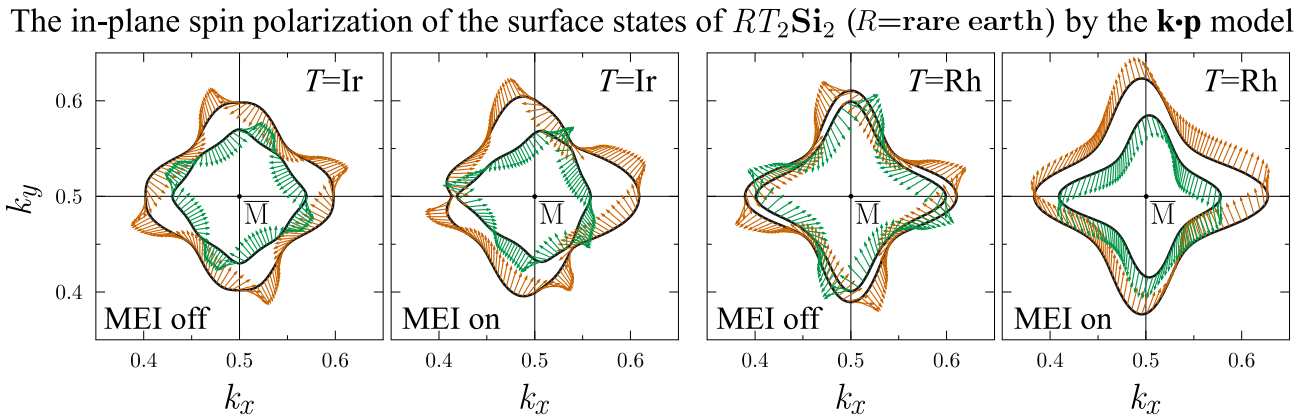

Figure 1. Spin-resolved FCs of the Si-terminated surface state of the compounds RT_2Si_2 with the in-plane orientation of the spins, $\langle \mathbf{S} \rangle = \langle S_x \rangle \hat{\mathbf{x}} + \langle S_y \rangle \hat{\mathbf{y}}$, indicated by green (orange) arrows for the inner (outer) contour. The shown FCs are obtained within a relativistic **k·p** six-band model without (MEI off) and with (MEI on) the magnetic exchange interaction of surface-state electrons with the 4*f* moments of the subsurface rare-earth atomic layer ferromagnetically ordered along the *y*-axis.