Spin-polarization of topologically protected edge states; DFT calculations and photoemission results

Gustav Bihlmayer

Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In the last years, the rapid development of the field of topological insulators was driven by a fruitful interplay of the theory of the electronic structure of these materials and experiments, mainly based on spin- and angle resolved photoemission spectroscopy (SP-ARPES) [1]. Not only the dispersion of the topological surface states agree usually between density-functional theory (DFT) and ARPES, also the helicity of the spin-orientations of the Dirac-cone and possible tiltings of the spin-directions are normally in good agreement. A comparison of the value spin-polarization remains, however, a delicate matter [2]. I will discuss several initial-state effects, e.g. from the vicinity of bulk-states or the probing-depth of the experiment. The latter can also influence the observed spin-polarization of bulk states in otherwise non-magnetic materials [3]. In addition, I will present results from many-body perturbation theory, which allow a more refined comparison to experiment.

[1] D. Hsieh et al., Science **323**, 919 (2009)
[2] C. Pauly et al., Phys. Rev. B **86**, 235106 (2012)
[3] A. Kimura et al., Phys. Rev. Lett. **105**, 076804 (2010)