DS 20: Topological Insulators: Status Quo and Future Directions (Joint session of DS, O and TT, organized by DS)

Time: Tuesday 12:30–13:00 Location: H8

DS 20.1 Tue 12:30 H8

Topological invariants in the embedding-potential — Hiroshi Ishida[2] and •Daniel Wortmann[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]College of Humanities and Sciences, Nihon University, Tokyo, Japan

The embedding potential[1] defined at the boundary of a semi-infinite crystal defines the boundary condition for the wavefunction and can be interpreted as its logarithmic derivative. We demonstrate how this embedding potential can be utilized to determine the Z_2 topological invariant in time-reversal invariant insulators and how the formation of the surface states can be understood in terms of properties of the embedding potential.

Besides the general ideas and the theory, numerical examples for simple topological insulators and trivial materials will be shown and compared.

[1] J.E.Inglesfield, J. Phys. C **14**, 3795 (1981)

DS 20.2 Tue 12:45 H8

Quantum-well stabilized two-dimensional topological crystalline insulators — Chengwang Niu, Patrick Buhl, •Gustav Bihlmayer, Daniel Wortmann, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

By means of density functional theory calculations, we find that monolayers of SnTe and PbTe can be characterized as two-dimensional topological crystalline insulators (2D-TCIs) with band gaps of 50 meV and 90 meV, respectively [1]. Embedded in NaCl or NaBr films, these 2D-TCIs are not only structurally stabilized, but also the band gaps can be enhanced up to 470 meV. Moreover, in these quantum-well structures the Madelung potential of the strongly ionic rocksalt lattice acting on the SnTe or PbTe layers enhances the band-inversion. Even in thicker, topologically trivial telluride films band-inversions can be induced that trigger a transition to a TCI state [2]. We further analyse the effect of an external magnetic (exchange) field on the SnTe and PbTe monolayers and find that the quantum anomalous Hall regime can be reached with fields exceeding 0.2 eV. This happens even for an in-plane oriented field where the mirror symmetry, protecting the TCI phase, is broken. We investigate the properties of the edge states for ribbons of different orientations using maximally localized Wannier functions.

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[1] C. Niu et al., Phys. Rev. B. **91**, 201401(R) (2015).
[2] C. Niu et al., submitted (2015).