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PhD position: Theoretical and experimental spectroscopic study of topologically non-trivial systems

Although many experimental methods give important information about the properties of complex and topologically non-trivial materials [1,2], photoemission spectroscopy, namely ARPES plays a crucial role in the approach to the microscopic origin of these properties. The goal of this project is to improve schemes for detection and qualifications of the topologically non-trivial materials by utilizing a combination of experimental data with state-of-the-art first principle photoemission calculations utilizing the one-step model of photoemission and density functional theory (DFT). Spin-polarized relativistic Korringa-Kohn-Rostoker (SPR-KKR) band structure software package [3,4] gives access to a photoemission signal with an accurate angular variation of ARPES spectral weight caused by an experimental geometry, photon energy and polarization state or surface termination [5-7]. Besides scrutinizing simple topological Weyl semimetals, we would like to disentangle a competing influence of the spin degree of freedom in materials with both strong spin-orbit coupling and magnetic order (e.g. in $MnBi_2Te_4$ [8]). The calculated spectra will be compared to experimental measurements of the observables of the photoemission experiment (photointensity, linear and circular dichroism, photoelectron spin-polarization, ...) and discussed in the context of topological properties – e. g. Berry flux monopoles or nodal lines identification in the band structure. This work will also benefit from a close collaboration with the photoemission theory group of Prof. Dr. Ján Minár at NTC, University of West Bohemia in Pilsen, Czech Republic (several scientific visits in Pilsen will be financed). The applicant will also have an opportunity of participating during the synchrotron beamtimes.

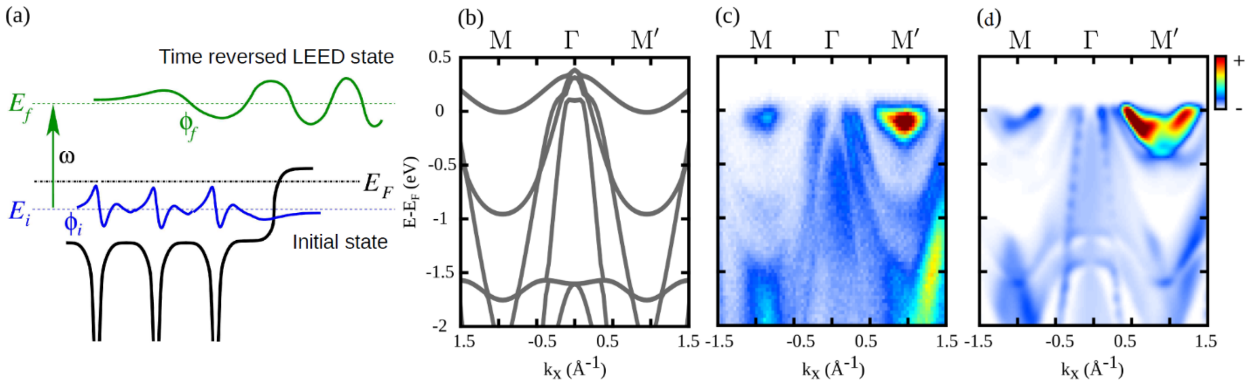

Figure 1: Information about a ground state band structure is not enough to properly account for spectral weight variation in the photoemission spectra. Implementation of surface-related effects, bulk sensitivity, temperature effects, matrix elements and final state effects (with the implementation of TR-LEED final state) in SPR-KKR package provides a reliable agreement of experimental and calculated photoemission spectra. Scheme of the photoemission transition from initial Bloch-like initial state into TR-LEED final state as implemented in SPR-KKR. (b) Theoretical ground state band structure of 1T-$TiTe_2$ along the M-Γ-M’ direction calculated by the QUANTUM ESPRESSO code. (c) Experimentally measured photoemission intensity using the same experimental geometry along the same cut with 21.7 eV photon energy and p-polarization obtained using the one-step model (KKR) method in (d). [6,9] (modified)

Position details: 1/2 x E13 (TVL) – 3.5-year contract starting on 1. 4. 2022, financed by the Center of Excellence ct.qmat

If you are interested, highly motivated and open for international collaborations, please contact

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Complexity and Topology in Quantum Matter

References:
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