Topological phases in II-VI semiconductor compounds: heterostructures and magnetically doped systems

Symmetry characteristics of solid-state crystals allow one establishing the number of independent parameters (invariants), to be determined experimentally or computationally, and which describe entirely thermodynamic and non-equilibrium properties of a given crystalline material. It has recently been demonstrated that this time-honoured view in not complete: it turns out that the magnitude of a functional over the set of Bloch wave functions (topological invariant) determines the topological class of the band structure, and that interfaces of materials belonging to different topological classes contain gapless boundary states showing worthwhile properties, such as protection against decoherence, the asset relevant to quantum computing.

Within this project, under guidance of my mentors Prof. Tomasz Dietl (supervisor) and Dr. Carmine Autieri (co-supervisor), I will employ state-of-the art fully relativistic first principle computational methods in order to elucidate the origin of surprising phenomena found experimentally in HgTe quantum wells that, along with WTe_2 atomically thin layers, represent a rather distinctive class of two-dimensional topological insulators. Furthermore, I will search by computer simulations for novel properties in new materials combinations of mercury chalcogenides and effects of their doping by magnetic impurities. My results, I suppose, will guide further materials developments and experimental efforts in my home institution, i.e., the International Centre for Interfacing Magnetism and Superconductivity with Topological Matter “MagTop” at the Institute of Physics, Polish Academy of Sciences, in which the mercury chalcogenide program is put forward in collaboration with the University of Rzeszów as well as with the Centre for Terahertz Technology Research and Applications “CENTERA” at the Institute of High Pressure Physics, Polish Academy of Sciences "Unipress".

Our three main objectives include:

1) Determination of the valence band structure in topological HgTe quantum wells, and finding out to what extent its complexity explains spectacular low-field quantization of the Hall resistance in the hole transport regime, as found experimentally in the University of Wuerzburg and by the MagTop/CENTERA collaboration.
2) Exploration of properties of HgTe/HgSe superlattices, particularly looking for quantum transitions from the phase of the topological semiconductor to the Weyl semimetal, and for new quantum transport phenomena associated with topological phase transformations.
3) Search for the nature of magnetic coupling between Cr magnetic impurities in Cr-doped HgTe and CdTe, and designing heterostructure architectures that will show the quantum anomalous Hall effect and hitherto unknown phenomena.

Our computational studies will be performed within the density functional theory by using the relativistic VASP package based on the plane wave basis set and a projector augmented wave (PAW) method. The modified Becke-Johnson exchange functional together with the local density approximation for the correlation functional will be employed. Within this approach, the determined magnitudes of the band gaps, as well as of spin-orbit splittings, are close to experimental values making our investigations of phase transitions valid quantitatively. Access to supercomputing facilities at the Interdisciplinary Center of Modeling, University of Warsaw, will be insured by separate grant applications for the CPU time.