Séminaire Friedhelm Bechstedt

Lundi 15 avril 2019 à 14h00

Salle réunion du LSI – salle 83-2034
Ecole polytechnique – Bâtiment 83

Quantum spin Hall phase versus quantized spin Hall conductivity?

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The quantum spin Hall (QSH) phase is a quantum state of matter, proposed to exist in two-dimensional (2D) semiconductors with inverted band structure and, hence, a character of a topological insulator (TI). Such a quantum phase should exhibit a spin Hall (SH) conductance but a vanishing charge Hall conductance. Since no external magnetic field is present, it can only be realized in materials with strong spin-orbit interaction (SOI). As central questions we investigate if the QSH phase is indeed characterized by a quantized static SH conductivity and how the answer depends on translational and point-group symmetry. As central quantities we study the SH conductivity $\sigma_{xy}(\omega)$ via the Kubo formula [1] and the Z^2 topological invariant via the parity method [2] by means of ab initio calculations of relativistic electronic structures of infinite 2D sheet crystals. The influence of the electronic-structure method is investigated. The third-rank tensor of the static SH conductivity is computed for three Z^2=1 classes: Hexagonal honeycomb atomic layers made by group-IV elements, germanene (Ge) and stanene (Sn), and their chemically functionalized, e.g. hydrogenated (GeH), iodinated (GeI) or fluoroinated (SnF), counterparts [3]. Square and rectangular 2D Bravais lattices are viewed for the model systems 1S- and 1T'-MoS2 as well as -WS2. In addition, dynamical results are given for atomically thin Ge-based systems [3]. The influence of destroying the inversion symmetry, e.g. by vertical electric fields, is discussed. The inverted band structures with a fundamental gap due to SOI are strongly modified by functionalization with I, F or H. As a consequence, we observe drastic changes in the frequency dependence of $\sigma_{xy}(\omega)$. For hexagonal 2D TIs the static SH conductivity for z-spin orientation exhibits quantization with e^2/h, the reciprocal von Klitzing constant, as shown in Fig. 1 [1,3]. This value is hardly influenced by temperature or Fermi level position. While for 2D square 1S crystals the quantization is less destroyed, the conductivity value tends to zero for rectangular 1T' systems. Lifting the inversion symmetry, the quantization is violated also for hexagonal sheets. We conclude that the QSH phase is not generally characterized by a quantized SH conductivity, only for high-symmetric cases.

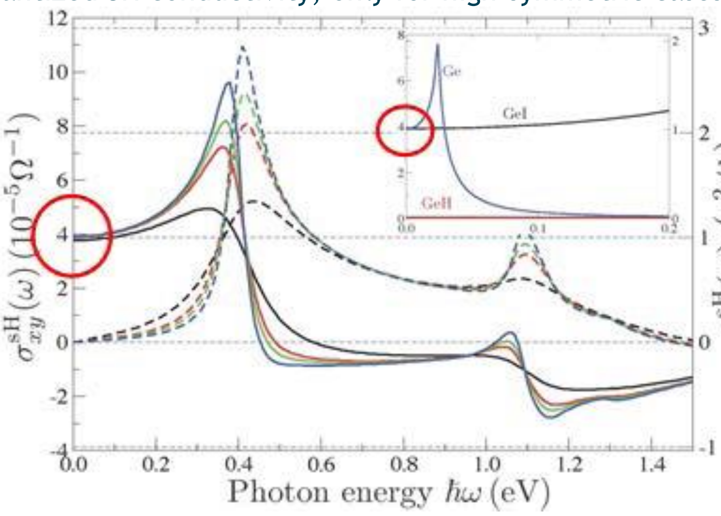

Fig. 1: Real (solid) and imaginary (dashed) part of spin Hall conductivity for Ge, GeI and GeH. [1] L. Matthes et al., Phys. Rev. B 94, 085410 (2016).[2] L. Fu and C.L. Kane, Phys. Rev. B 76, 045302 (2007).[3] L. Matthes et al., Phys. Rev. B 93, 121106 (R) (2016).[4] F. Matusalem et al., submitted to PRL

Pause café à 13h30