INVITATION
to a joint Seminar on
Theoretical Chemistry and
Materials Sciences

Monday, January 8th 2018, 16:00 hours
in PHY 5.0.21

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Ab-initio investigations of 2D Dirac materials:
graphene and topological insulators

In the last decade, Dirac materials emerged as promising candidates for the development of functional devices at the nanoscale. These materials possess a unique Dirac-like cone type of low-energy band structure within the first Brillouin zone. In this work, we will study two types of Dirac materials as possible candidates for nanoelectronic applications: graphene and bismuth telluride based topological insulator materials. Regarding the possible use of graphene in electronic nanodevices, it is crucial to achieve an optimal contact between graphene and bulk materials (i.e. the electrode). Most commonly, two possible ways are proposed to connect graphene to bulk material such as metals: the more conventional side contact geometry and the rather novel edge contact conformation.

The role of the homogeneity and of edge contaminations on the transport properties of both contact geometries are investigated in this work. Topological insulators (TIs) possess a topological surface state (TSS) that is protected by time reversal symmetry (TRS). In collaboration with experimentalists, the influence of magnetic impurities on the properties of the TSS of novel TI materials is investigated in this project.

Host: Dr. David Egger