Properties of transition metal ions in wide-gap semiconductors and three-dimensional topological insulators: Description for the general public

In the project, transition metal (TM) ion in solids means the single atom/impurity, which varies from surrounding atoms of the host material. The properties of such ion strongly depend on environment, *i.e.* they are generally different in metals, semiconductors or insulators.

In solids, some electrons which initially belong to the uncharged (free) atom form chemical bonds with surrounding atoms in the crystal. These electrons may be still localized in the closeness of such atom, transfered to the neighboring ones or exist 'somewhere between'. Some electrons, like conduction electrons in metals, may even move freely in the crystal. Therefore, we use the name 'ion' rather than 'atom' when referring to the solids and we also use the name 'impurity' or 'dopant' when referring to the atom different from all around.

As a consequence of bond forming, the transition metal ions can exist in different oxidation state, which means different number of electrons around such impurity, and in various spin configurations. These properties strongly affect the characteristics of the doped material. Especially, TM ions can change the structural, electronic and/or magnetic properties of the host crystal. Therefore, doping is known as one of the most efficient methods for tuning the physical and chemical properties of solids and hence it has a decisive impact on the possible application of many future materials.

The objective of the project is theoretical investigation of properties of TM ions in semiconductors (like ZnO) and topological insulators (like Bi_2Se_3). These materials exhibit fascinating physical properties, and in all of them TM ions play a role of high importance. The presence of TM ions in ZnO changes its optical properties and we want to know 'why?'. Bi_2Se_3 exhibits a new state of matter named 'topological insulator', *i.e.* it behaves as an insulator but its surface contains metallic states. Doping Bi_2Se_3 by TM is intensively studied, since it may lead to observation of the quantum anomalous Hall effect (in which electron transport along the edges of the sample occurs without dissipation) or topologically protected superconducting state (in which the Cooper pairs – carriers of superconducting current coexist with Majorana fermions - particles identified with their own anti-particles). Our aim is to obtain the properties of such TM ions and to explain their influence on topological state of Bi_2Se_3.

Therefore, the project has an impact on the area of the first principle calculations for solids containing TM impurities. The made attempt to describe TM elements in solids is expected to help in searching new combinations of TM ions and hosts materials with the desired structural, electronic or magnetic properties. Therefore, our project is not only supposed to stimulate a further development of fundamental research in the field of semiconductors and topological insulators, but also the production and device application involving TM doped materials.