

PREDICTION AND DISCOVERY OF TOPOLOGICAL MATERIALS: WANNIER CHARGE CENTERS AND Z2PACK PACKAGE

Topological phases can be found in many weakly interacting crystalline materials, the electronic structure of which is easily accessible with *ab initio* software packages like ABINIT. Unlike the metal from insulator distinction accessible from the band structure – eigenvalues of the crystalline Hamiltonian, all the geometrical and topological properties of the material is stored in the eigenstates of the crystalline Hamiltonian – the Bloch states.

In this talk I will describe how this information can be extracted from standard first-principles calculations and used for prediction of topological phases hosted in insulators and metals. Time permitting, I will also describe novel software tools, applicable with ABINIT, that allow for a complete *ab initio* description of non-trivial topological phases of materials.