SPIN-ORBIT INTERACTION —
A PATH TO TOPOLOGICAL MATTER IN REAL AND MOMENT SPACE

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The spin-orbit interaction is a small and seemingly unimportant interaction in solids, but plays in fact a crucial role in relating the properties of the electron spin to the underlying lattice, subsequently lifting electron degeneracies, generating many spin-dependent transport phenomena, e.g. spin-orbit torque or spin-Hall effect, and making magnets of practical use as well as of commercial interest. It is at the origin of currently studied quantum materials exhibiting topologically protected states in momentum space, e.g. topological insulator and Weyl semimetals, as well as in reals space, such as skyrmions and bobbers in chiral magnets witnessing localized curling magnetic spin textures.
In this presentation I show examples where this field benefits from innovative developments of electronic structure methods (FLEUR, and KKRnano) in combination with cutting edge applications on high-performance computers. I show examples of describing large skyrmions using a scale-bridging approach between DFT and a spin-lattice model, calculating the electronic structure of small skyrmions in unit cells of a few thousand atoms, describing spin-dependent transport properties using mixed Berry phases and band-gaps of topological insulators using relativistic GW.