Abstract for the general public

Magnetism is a widespread phenomenon that has a major place in our everyday life. Magnetic materials are ubiquitous, included in all our technological devices, as well as in many industrial products. Speakers, power transformers, wind turbines, computers, and medical machines are just a few examples of things that characterize our life and that would not be available without magnetism. Hence, it is not surprising that much research in condensed matter physics is focused on magnetism, magnetic materials, and their applications. While traditionally most attention has been focused on bulk materials, in the last two decades more complex systems have been under intense scrutiny, including magnetic surfaces, interfaces, thin films, multilayers and even two-dimensional materials. Experimental progresses on the observation and manipulation of single atoms made it possible to probe magnetic interactions directly at the atomic scale, which has opened new perspectives for engineering single-atom magnets and magnetic nanostructures.

Despite these intriguing promises, the ground-breaking experimental advances in synthesis, characterization and atomic manipulation have not been accompanied by an adequate leap in theoretical understanding. A crucial challenge is that the theoretical description of magnetic behavior requires the solution of problems at very different length (and time) scales. Magnetic interactions originate at the atomic scale, so their description requires the quantum-mechanical solution of a many-body problem of interacting electrons. The long-range magnetic order, however, arises at a much larger length scale, making a direct quantum-mechanical approach to the full problem unfeasible. Multiscale methods have then become the state-of-the-art to describe magnetic properties of complex composite materials, although at the price of important approximations.

The scientific goal of the present project is to investigate the role played by the anisotropy of the magnetic coupling in the emergence of magnetism in a variety of rare-earth based systems, ranging from bulk metals to adatoms on selected substrates. In our approach, the electronic and magnetic properties will be investigated directly at the atomic scale, using state-of-the-art electronic structure methods, based on density-functional theory (DFT) and dynamical mean-field theory (DMFT). The formation of the magnetic order at the nanoscale will be investigated by means of atomistic spin dynamics simulations, which require the results of the other calculations as input. This multi-scale approach will provide a very accurate description of the systems at hand and will clarify the very nature of rare-earth magnetism. The scientific results obtained in this project will not only improve our understanding of the control of the magnetic coupling directly at the atomic scale, but will also favour the transition towards better materials for spintronics, quantum computation and permanent magnets.