A computational approach to the microscopic modeling of magnetic insulators

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Low-dimensional quantum magnets exhibit a variety of exotic magnetic behaviors and unusual ground states, as revealed by the growing number of experimental reports. However, the analysis of the experimental data is often impeded by the complexity of the underlying magnetic model, while the large number of free parameters gives rise to ambiguous solutions.

Recent development of computational techniques and facilities turned DFT calculations into a powerful method to evaluate the model parameters on the microscopic level. This approach is based on DFT band structure and total energy calculations, and can be applied to a wide range of magnetic insulators.
The methodological issues and the details of the computational procedure will be discussed in the first part of the talk. The magnetically active orbitals and relevant couplings can be reliably estimated using conventional DFT methods, while the Wannier functions technique allows to treat systems featuring more than a dozen of magnetic orbitals. A complementary approach is based on total energy calculations for magnetic supercells, which require more sophisticated approaches, such as DFT+U or hybrid functionals. I will put a particular emphasis on the case of noncollinear magnetic arrangements, which can be used to evaluate anisotropic exchange parameters.

In the second part, several examples will be presented. I will compare our computational results for representative systems with the available experimental data. It will be shown that the choice of the functional (different DFT+U methods or hybrid functionals) for total energy calculations often plays a crucial role. Accuracy issues and possible extensions of the computational procedure will be addressed as well.

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