O.23 Developments of second principle spin models and lattice-electron models

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We present some recent developments regarding (i) spin models, (ii) the lattice models based on Lattice Wannier Functions (LWF), and (iii) the electron-lattice coupled models developed in a second-principles framework. Regarding spin models, during the past two years, we have made a lot of progress in the automated building of second-principles Heisenberg-like Hamiltonians from first-principles data. First, there are several new features in TB2J, the Python package for computing the exchange parameters from tight-binding electron Hamiltonians using Green's function method. First, beyond the input from Wannier functions, we can also use numerical atomic orbitals, e.g. from the SIESTA and OpenMX codes. Second, the Dzyaloshinskii-Moriya interactions and the anisotropic exchange can now be calculated from the non-collinear spin DFT results, in addition to the isotropic exchange previously implemented. Third, the package is designed to minimise the user input which make it suitable for automatic workflows. As such, we have also developed a prototype of high-throughput workflow for the simulation of magnetic properties, from DFT calculations to the building the spin Hamiltonian, and finally the spin dynamics simulation. We'll also discuss the implementation of the coupled spin-lattice dynamics in MULTIBINIT.

Regarding lattice models, MULTIBINIT relies on a method including all individual atomic displacements and strains. However, sampling the whole Born-Openheimer energy surface and parametrising such models is not always easy when there are many degrees of freedom and the interactions are strongly anharmonic. One way to simplify the problem is to use lattice effective Hamiltonians as pioneered during the 90's and restricting to a relevant subspace of atomic displacements described using LWF. We have built an easy-to-use tool for the construction of LWF's and the corresponding harmonic potentials by unfolding the inter-atomic force constants. The tools for adding anharmonic LWF potentials (essential when treating systems with structural instabilities) and performing LWF dynamics are also under development, providing an alternative easy access the large-scaled and physically transparent simulations of the lattice dynamics with MULTIBINIT when few degrees of freedom have to be considered.

Finally we have also developed a method for modeling systems with coupled electron and lattice degree of freedoms. We will discuss first how to model the lattice degree of freedom at distinct levels considering either the full set of phonons, or a selected branches of phonons, or even only few selected phonon modes. The former two approaches correspond to the use of LWF or individual patterns of displacements. We will discuss then how to treat the electronic degrees of freedom using either a Wannier-function-based tight-binding or Hubbard model. Then the electron lattice coupling can be added to the model. We will demonstrate the usefulness of such a coupled LWF-electron model to tackle the metal insulator transition in VO_2.

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