Spin dynamics in Multibinit

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Atomistic spin dynamics has been implemented in Multibinit for modeling large-scale spin systems. The formalism is based on a Heisenberg model, which includes exchange and Dzyaloshinskii-Moriya interactions, single ion anisotropy, dipole-dipole interaction, and an external magnetic field. The dynamics is performed using the Landau-Lifshitz-Gilbert (LLG) equation [1].

A program has been developed to handle the automatic calculation of superexchange interaction parameters J of all neighbors through a Wannier function (WF) based tight-binding Hamiltonian built from density functional theory. The spin rotation of localized WFs is treated perturbatively, allowing for the calculation of exchange parameters thanks to the spin force theorem [2].

We also discuss the ongoing development of a coupled spin-lattice dynamics. The coupling between the lattice and spin subsystems is considered, and the molecular dynamics and spin dynamics are performed simultaneously.

References

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