The MULTIBINIT software project

J. Bieder, A. Martin, M. M. Schmitt, F. Ricci, C. Garcia-Castro, He Xu, N. Helbig, W. Lafargue-dit-Hauret, E. Bousquet, M. Verstraete and Ph. Ghosez
CESAM, University of Liège
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The atomic-scale description of mesoscopic systems at finite temperatures still remains very challenging, and significant efforts have been devoted recently to the development of second-principles effective models. These extend the capabilities of DFT calculations to larger systems and time-scales, while retaining most of the first-principles predictive power and accuracy.

The purpose of the MULTIBINIT software project is to develop a unified platform for the automatic construction of “second-principles” effective models for atoms, electrons, lattice modes and spin degrees of freedom, and for their use in mesoscopic simulations, either separately or coupled together (e.g. atoms + electrons, atoms + spins, lattice mode + spins).

In this talk, we will first provide an overview of the generic structure of MULTIBINIT and of the present status of development of the different types of models. Then, we will provide a more detailed description of the lattice part [1], providing some details of the implementation and highlighting the limitations of the present version. A few words will be said regarding the improvements of the AGATE post processing tool, and the features available for the analysis of MD runs, phonons, etc... More detailed descriptions of the electron, spin and lattice mode parts will be provided in separate presentations.

*[1] J. C. Wojdel, P. Hermet, M. P. Ljungberg, Ph. Ghosez and J. Iniguez, J. Phys. Condens. Matter **25**, 305401 (2013).*