Construction of complex Effective Lattice Models with MULTIBINIT and Electron-Phonon Couplings combining MULTIBINIT & SCALE UP

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The lattice part of MULTIBINIT relies on the construction of effective atomic models, integrating out the electronic degrees of freedom and properly mimicking the Born-Oppenheimer energy surface around a given reference configuration [1]. In practice, the energy is expressed in terms of individual atomic distortions and macroscopic strains by means of a Taylor series. MULTIBINIT automatically generate the terms allowed by symmetry up to a given order and range of interactions and then determine the values of the related coefficients from a set of first-principles data. Nonetheless, the automatic generation of models for materials with complex energy surface incorporating multiple local minima and large distortions with respect to the reference still pose significant problems. The greatest challenge is to guarantee the boundedness of the model i.e. avoid divergence of the model energy to minus infinity for large lattice distortion amplitudes in the high-dimensional space of the individual atomic distortions. Here, we present a simple algorithm that imposes the boundedness for any given effective potential while keeping its precision to a limited range of first-principles data. The successful application of this algorithm to the case of $CaTiO_3$ is discussed.
Then, it is sometimes important or even necessary to reintroduce explicitly some electronic degrees of freedom in the simulation. This can be achieved by combining the lattice part of MULTIBINIT with a second-principles model describing the relevant electronic states, while avoiding double counting as provided by SCALE-UP [2]. We will show the first implementation of a coupled electron-lattice models obtained from the combination of MULTIBINIT with the SCALE-UP module responsible for the electron treatment. The technical aspects of the implementation will be introduced and its capabilities exemplified on a simple electron-lattice model addressing fundamental questions of orbital physics in solids.

Finally, an outlook of future challenges of the joint MULTIBINIT SCALE-UP project - further integration of data structures, code licensing-distribution, integrated testing - will be made and posed to discussion.

[1] J. C. Wojdel, P. Hermet, M. P. Ljunberg, Ph. Ghosez and J. Íñiguez, J. Phys.: Condens. Matter 25, 305401 (2013).
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