EFFECTIVE HAMILTONIAN APPROACH AND MULTIBINIT PACKAGE ASSOCIATED FOR STUDYING STRUCTURAL PHASE TRANSITIONS

W. Lafargue-dit-Hauret[1], E. Bousquet[1] and Ph. Ghosez[1]

[1]Physique Théorique des Matériaux, Université de Liège, B-4000 Sart Tilman, Belgium

First principles calculations provide an extremely accurate understanding of microscopic mechanisms which govern structural phase transitions in solid state materials. For instance, density functional theory allows to capture the origin of ferroelectricity in high symmetry phases of perovskite oxides. Even with the spectacular improvement of computational facilities and algorithm advances in the past decade, *ab-initio* molecular dynamics still remain challenging to simulate finite-temperature structural transitions, requiring large size and time scales. To tackle this inconvenience, an effective Hamiltonian approach acting in a restricted subspace of phonon branches and parametrized from first principles was proposed during the 90's [1,2]. Then, more recently, a generalization of this method [3], including all ionic degrees of freedom, was proposed and implemented in MULTIBINIT.

Here, we present the implementation within MULTIBINIT of a method projecting the all-atoms model within the restricted subspace spanned by one local lattice mode (or a lattice Wannier function) as done in the original effective Hamiltonian approach. Being able within MULTIBINIT to build together, on the same set of first-principles data, an all-atom model and its projection within a restricted subspace will be useful to investigate further the interplay of the soft mode with other phonon modes in displacive materials and also to build simplified spin-lattice models.

References

[1] W. Zhong, D. Vanderbilt and K. M. Rabe, Phys. Rev. B **52**, 6301 (1995).

[2] R. D. King-Smith and D. Vanderbilt, Phys. Rev. B **49**, 5828 (1994).

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