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Computing ab initio free energy contributions of point defects B. GRABOWSKI, Max-Planck-Institut Duesseldorf, L. ISMER, T. HICKEL, J. NEUGEBAUER — A common assumption when computing defect concentrations is that the dominant entropy contribution is due to configurational entropy. Other entropy contributions such as harmonic and anharmonic lattice vibrations are assumed to be second order effects and are computationally expensive to calculate. Thus, such contributions have been rarely considered in defect calculations. With the increasing capability of ab initio approaches to e.g. provide accurate free energies to macroscopic approaches (e.g. CALPHAD), the inclusion of the aforementioned smaller entropy contributions will become more and more important. We have therefore developed a hierarchical scheme to coarse grain the configurations space allowing to efficiently calculate harmonic and anharmonic contributions to vacancy formation [PRB 79, 134106 (2009)]. In the present talk we will discuss the application of this approach to vacancies in aluminum. It turns out that the entropy of vacancy formation is significantly affected by anharmonicity.

Blazej Grabowski
Max-Planck-Institut Duesseldorf

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