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Ab initio up to the melting point: Anharmonicity and vacancies in aluminum B. GRABOWSKI, L. ISMER, T. HICKEL, J. NEUGEBAUER, Max-Planck-Institut Düsseldorf, Germany — At elevated temperatures, the heat capacity of metals strongly deviates from the harmonic prediction. This was pointed out long ago[1] and various explanations have been considered. Ab initio calculations showed[2] that a dominant part can be explained by quasiharmonic excitations. However, the *detailed* balance of further contributions, such as explicit anharmonicity and vacancies, is not clarified yet even for simple elementary metals. Aluminum is a prototypical example. Even though intensively studied, the ambiguous experimental situation has made a classification of the mechanisms impossible. To resolve the situation, we have calculated the full volume and temperature dependent *ab initio* free energy surface employing density-functional theory. In particular, we have included anharmonic and vacancy contributions using numerically highly efficient methods to coarse grain the configuration space. To obtain accurate vacancy energies, we have included the full spectrum of excitations: quasiharmonic, electronic, and explicitly anharmonic. The results are in contradiction to common belief, nevertheless the essential physics can be captured by a simple model.

[1]M. Born and E. Brody, Zeitschrift für Physik 6, 132 (1921)
[2]B. Grabowski, T. Hickel, J. Neugebauer, Phys. Rev. B 76, 24309 (2007)

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