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The intrinsic defect structure of $Al_{1-x}B_2$

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The *ab initio* calculation of phase diagrams is still in its very early stages. For an outset towards new developments, we have chosen the simple hexagonal system AlB_2, which is nevertheless very interesting due to its close relation to the high-temperature superconductor MgB_2. Up to now, the synthesis of stoichiometric AlB_2 has been impossible. Grown in an aluminium flux, a composition between $Al_{0.9}B_2$ (from X-ray refinement) and $Al_{0.85}B_2$ (from mass-density measurements) has been found [1]. So far, a microscopic explanation for this defect structure has been missing. Here, we present DFT band structure calculations within the local density approximation to investigate the structural stability in the phase equilibrium $AlB_2 \Leftrightarrow Al_{1-x}B_2 + Al_x$. The calculations are carried out using a full-potential local-orbital scheme (FPLO) [2]. The defects are treated using the coherent potential approximation (CPA) [3]. Taking into account the full lattice relaxation depending on the defect concentration x, we find a stable energy minimum for the composition $Al_{0.87}B_2$. This is in excellent agreement with the experimental findings and explains the nonstoichiometric composition of present AlB_2 samples. In contrast to the complex influence of the defects to the phase diagram, the defect-related electronic properties can be essentially understood within a simple rigid band model.

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