The intrinsic defect structure of \( \text{Al}_{1-x}\text{B}_2 \)

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The \textit{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\(_2 \leftrightarrow \text{Al}_{1-x}\text{B}_2 + \text{Al}_x\). 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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