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Electrons and phonons in the hexagonal layered superconducting alloy $CaAl_{2-x}Si_x$ GIOVANNI B. BACHELET, INFM and Dipartimento di Fisica, Università "La Sapienza", I-00185 Roma, Italy, LILIA BOERI, Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany, MATTEO GIANTOMASSI, UPCPM, Université Catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium —
We report a first-principles study of structural, electronic and vibrational properties of the superconducting C_{32} phase of the ternary alloy $CaAl_{2-x}Si_x$, both in the experimental range of stability, $0.6 \leq x \leq 1.2$, and outside, in the limits of high Al and high Si concentration. We find that the dependence of the electronic bands on composition is well described by a rigid-band model, which breaks down outside the experimental range of stability. This breakdown, in the limit of high Al concentration, is connected to vibrational instabilities, and results in important differences between $CaAl_2$ and MgB_2. Unlike MgB_2, the interlayer band and the out-of-plane phonons play a major role on the stability and superconductivity of CaAlSi and related C_{32} intermetallics.

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