

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Sorting Category: 05.11.1 (C)

Electrons and phonons in the hexagonal layered superconducting alloy $\text{CaAl}_{2-x}\text{Si}_x$ GIOVANNI B. BACHELET, INFN 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 $\text{CaAl}_{2-x}\text{Si}_x$, 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.

Prefer Oral Session
 Prefer Poster Session

Giovanni B. Bachelet
Giovanni.Bachelet@roma1.infn.it
INFN and Dipartimento di Fisica,
Università “La Sapienza”, I-00185 Roma, Italy

Date submitted: 26 Nov 2005

Electronic form version 1.4