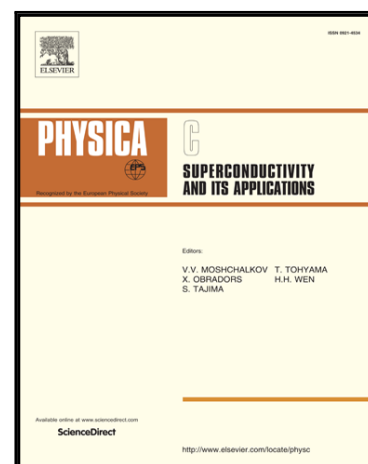


Accepted Manuscript

First principles predictions of electronic and elastic properties of BaPb_2As_2 in the ThCr_2Si_2 -type structure

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PII: S0921-4534(17)30432-X
DOI: [10.1016/j.physc.2017.10.013](https://doi.org/10.1016/j.physc.2017.10.013)
Reference: PHYSC 1253207



To appear in: *Physica C: Superconductivity and its applications*

Received date: 28 August 2017
Revised date: 18 October 2017
Accepted date: 26 October 2017

Please cite this article as: Y. Bourourou , S. Amari , I.E Yahiaoui , B. Bouhafs , First principles predictions of electronic and elastic properties of BaPb_2As_2 in the ThCr_2Si_2 -type structure, *Physica C: Superconductivity and its applications* (2017), doi: [10.1016/j.physc.2017.10.013](https://doi.org/10.1016/j.physc.2017.10.013)

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Highlights

- The equilibrium lattice parameter a agree well with the experimental data while the c/a ratio is far away from the experiment.
- The calculated elastic constants suggest that BaPb_2As_2 is very soft material and mechanically stable.
- The BaPb_2As_2 can be classified as ductile since B/G is larger than 1.75 and ν is larger than 0.25.

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