

Accepted Manuscript

Insight into the physical properties of two niobium based compounds, Nb_3Be and Nb_3Be_2 , via a first principles calculation

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PII: S0577-9073(18)30173-4
DOI: [10.1016/j.cjph.2018.05.016](https://doi.org/10.1016/j.cjph.2018.05.016)
Reference: CJPH 538



To appear in: *Chinese Journal of Physics*

Received date: 31 January 2018
Revised date: 7 April 2018
Accepted date: 4 May 2018

Please cite this article as: Zahidur Rahaman Md , Lokman Ali Md , Insight into the physical properties of two niobium based compounds, Nb_3Be and Nb_3Be_2 , via a first principles calculation, *Chinese Journal of Physics* (2018), doi: [10.1016/j.cjph.2018.05.016](https://doi.org/10.1016/j.cjph.2018.05.016)

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Highlights

- The physical properties of Nb_3Be and Nb_3Be_2 have been studied.
- The Nb_3Be phase is more ductile than the Nb_3Be_2 phase.
- The Nb_3Be_2 phase is harder than the Nb_3Be phase.
- The Nb_3Be phase is more conducting than the Nb_3Be_2 phase.
- The Nb_3Be_2 phase is electrically more stable than the Nb_3Be phase.

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