

Accepted Manuscript

Structural, mechanical, electronic and thermal properties of the newly predicted NB_2 from ab initio calculations

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PII: S0577-9073(17)30001-1
DOI: [10.1016/j.cjph.2017.08.029](https://doi.org/10.1016/j.cjph.2017.08.029)
Reference: CJPH 341



To appear in: *Chinese Journal of Physics*

Received date: 1 January 2017
Revised date: 20 August 2017
Accepted date: 28 August 2017

Please cite this article as: M.A. Alam , M. Nuruzzaman , M.A.H. Shah , F. Parvin , M.A.K. Zilani , Structural, mechanical, electronic and thermal properties of the newly predicted NB_2 from ab initio calculations, *Chinese Journal of Physics* (2017), doi: [10.1016/j.cjph.2017.08.029](https://doi.org/10.1016/j.cjph.2017.08.029)

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Highlights

- $t\text{-NB}_2$ is a newly predicted superhard material with Vickers hardness 43-54 GPa.
- $t\text{-NB}_2$ exhibits both mechanical and thermodynamic stability.
- Debye and melting temperatures reveal the strong microhardness of $t\text{-NB}_2$.
- DOS and Mulliken populations predict strong covalent bonding of B-B(B-N) atoms.

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