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Ab-initio Study of the Properties of Advanced Metal Nitrides M2N3 (where M = Ta, V, Nb)

The structural, elastics, and electronic properties of the advanced metal nitrides M2N3 and their ternary phases are investigated using ab-initio plane wave pseudopotentials under the framework of density functional theory. The relative stability of the ternary phases were also computed. Results obtained were compared with the available experimental and theoretical data.

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