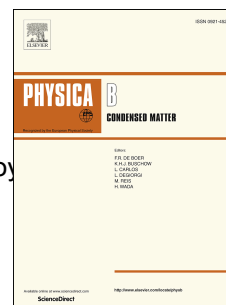


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# Structural, elastic and electronic properties of typical NdMgT<sub>4</sub> (T=Co, Ni, Cu) alloys from *ab initio* calculation

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## ABSTRACT

The crystal structure, elastic and magnetic properties of important ternary Mg-based alloys NdMgT<sub>4</sub> (T=Co, Ni, Cu) have been studied using reliable *ab initio* calculations. Both cohesive energy and charge density difference suggest that three alloys have good structural stability with the order: NdMgCo<sub>4</sub> > NdMgNi<sub>4</sub> > NdMgCu<sub>4</sub>. It shows that NdMgCo<sub>4</sub> alloy has magnetic moments with the Co atoms being the main contribution, which is also in agreement with the calculated electronic structures. We find that NdMgT<sub>4</sub> (T=Co, Ni, Cu) alloys are all ductile materials with bulk-to-shear modulus (B/G) values higher than 1.75. The trends of calculated values for the shear moduli C<sub>s</sub> and C<sub>44</sub> are consistent with that of shear modulus G and young's modulus E, proving

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