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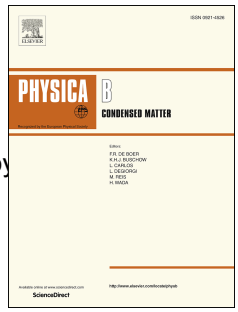

Structural, elastic and electronic properties of typical $NdMgT_4$ (T□=□Co, Ni, Cu) alloy from *ab* initio calculation

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Structural, elastic and electronic properties of typical $NdMgT_4$ (T=Co, Ni, Cu) alloys from *ab* initio calculation

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A B S T R A C T

The crystal structure, elastic and magnetic properties of important ternary Mg-based alloys $NdMgT_4$ (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: $NdMgCo_4$ > $NdMgNi_4$ > $NdMgCu_4$. It shows that $NdMgCo_4$ 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 $NdMgT_4$ (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_s and C_{44} are consistent with that of shear modulus G and young's modulus E, proving

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