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Structural, Elastic, Electronic and Magnetic Properties of the full Heusler Compound Ti_2NiX $X = (Al, Ga \text{ and } In)$

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In this article we will study the structural, elastic, electronic and magnetic properties of new Ti₂-based Heusler alloys Ti_2NiX ($X = Al, Ga \text{ and } In$), using ab initio electronic structure calculations. The results show that these compounds exhibit a half-metallic behavior. The full-Heusler alloys show a Slater-Pauling behavior and the total spin magnetic moment per unit cell (M_t) following the rule $M_t = Z_t - 24$. The origins of the gap in these half-metallic alloys are well understood. It is found that the half-metallic properties of Ti₂-based compounds are insensitive to the lattice distortion and a fully spin polarization can be obtained within a wide range of lattice parameters. Calculations of the total magnetic moment is $3.00 m_B$ for a wide range of mesh. Our results suggest that Ti_2NiX ($X = Al, Ga \text{ and } In$) are promising materials for spintronics applications in the future This is favorable in practical application.