

Ferromagnetic 1D Ti atomic chain

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Using the Full potential linearized augmented plane wave (FLAPW) method, we have explored the magnetic properties of one dimensional Ti atomic chains. It has been obtained that the unsupported 1D Ti atomic chain has ferromagnetic ground state with magnetic moment of 1.88 Bohr magneton. Very interestingly, the ferromagnetic ground state is maintained even on NiAl(110) surface and the calculated magnetic moment is 1.24 Bohr magneton. We have also performed magnetic anisotropy of 1D Ti/NiAl(001). We have realized that the magnetization aligns along the chain axis and the magnetic dipolar interaction is dominant in determination of magnetization direction, not the magnetocrystalline anisotropy arising from spin-orbit interaction.