

Half Metallic Antiferromagnetic of Doped TiO₂ Rutile with Doubles Impurities (Os, Mo) from Ab Initio Calculations

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Abstract : Electronic and magnetic calculations based on density functional theory within the generalized gradient approximation for II-VI compound semiconductor TiO₂ doped with single impurity Os and Mo; these compounds are a half metallic ferromagnet in their ground state with a total magnetic moment of 2 μ_B for both systems. Then, TiO₂ doped with double impurities Os and Mo have been performed. As result, Ti_{1-2x}Os_xMo_xO₂ with $x=0.065$ is half-metallic antiferromagnets with 100% spin polarization of the conduction electrons crossing the Fermi level, without showing a net magnetization. Moreover, Ti₁₄OsMoO₃₂ compound is stable energetically than Ti_{1-x}Mo_xO₂ and Ti_{1-x}Os_xO₂. The antiferromagnetic interaction in Ti_{1-2x}Os_xMo_xO₂ system is attributed to the double exchange mechanism, and the latter could also be the origin of their half metallic.

Keywords : diluted magnetic semiconductor, half-metallic antiferromagnetic, augmented spherical wave method

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