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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 μB for both systems. Then, TiO2 doped with double impurities Os and Mo have been performed. As result, Ti1-2xOsxMoxO2 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 Ti1-xMoxO2 and Ti1-xOsxO2. The antiferromagnetic interaction in Ti1-2xOsxMoxO2 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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