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First-Principles Study of Electronic and Magnetic Properties of Half-Metallic Fe_2MO_4 Alloys (M=Fe, Co and Ti)

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A systematic study on electronic structure and magnetic properties of binary and ternary spinel Co- and Ti-substituted Fe_3O_4 is presented by the first-principles pseudo-potential method. Total energy calculations are taken into account for both the inverse and normal spinel structures as well as the atomic arrangement of substitutional elements in order to find out ground state phase for all the systems. Fe_2CoO_4 and Fe_2TiO_4 were calculated to be ferromagnetic half-metallic, but Fe_3O_4 to be ferrimagnetic half-metallic. The electronic band gaps of the ternary alloys are broader than that of the binary. Being consistent with experiments, calculated spin moments of 8 μB/f.u. of ternary alloys are much larger than that (4 μB/f.u.) of Fe_3O_4 due to the magnetic structures. We will also discuss on magnetocrystalline anisotropy energy and elastic property under tetragonal lattice distortion, in orderto elucidate physical origin of experimentally observations of quite large magnetostrictions of the ternary alloys but very small one of the binary alloy.