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Polyanion Driven Antiferromagnetic and Insulating Ground State of Olivine Phosphates: $LiMPO_4$.[1] AJIT KUMAR JENA, B. R. K. NANDA, Indian Inst of Tech-Madras, CONDENSED MATTER THEORY COMPUTATION TEAM — Through density functional calculations we have investigated the electronic and magnetic properties of $LiMPO_4$, where M is a 3d transition metal element. We find that contrary to many transition metal oxides, in these Olivine phosphates the band gap is originated due to crystal field anisotropy as well as weak O-p – M-d covalent interaction. Both of them are attributed to the presence of PO_4^{3-} polyanion. The anisotropic crystal field, in the absence of covalent interactions, creates atomically localized non-degenerate M-d states and therefore the gap is a natural outcome. Onsite repulsion, due to strong correlation effect, further enhances the gap. These localized d states favor high-spin configuration which leads to antiferromagnetic ordering due to Hund's coupling. Experimentally observed low Neel temperature of this family of compounds is explained from the DFT obtained spin exchange interaction parameters.

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