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Magnetism in Olivine-type $LiCo_{1-x}Fe_xPO_4$ Cathode Materials: Bridging Theory and Experiment VIJAY SINGH, YELENA GERSHINSKY, MONICA KOSA, MUDIT DIXIT, DAVID ZITOUN, DAN THOMAS MAJOR, Department of Chemistry, Bar-Ilan University, Ramat-Gan, Israel, DR. DAVID ZITOUN COLLABORATION — We present a non-aqueous sol-gel synthesis of olivine type $LiCo_{1-x}Fe_xPO_4$ compounds (x = 0.00, 0.25, 0.50, 0.75, 1.00). The magnetic properties of the olivines are measured experimentally and calculated using first-principles theory. Specifically, the electronic and magnetic properties are studied in detail with standard density functional theory (DFT), as well as by including spin-orbit coupling (SOC), which couples the spin to the crystal structure. We find that the Co^{2+} ions exhibit strong orbital moment in the pure $LiCoPO_4$ system, which is partially quenched upon substitution of Co^{2+} by Fe^{2+}. Interestingly, we also observe a non-negligible orbital moment on the Fe^{2+} ion. We underscore that the inclusion of SOC in the calculations is essential to obtain qualitative agreement with the observed effective magnetic moments. Additionally, Wannier functions were used to understand the experimentally observed rising trend in the Néel temperature, which is directly related to the magnetic exchange interaction paths in the materials. We suggest that out of layer M – O – P – O – M magnetic interactions ($J_\perp$) are present in the studied materials.

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