Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic supplementary information (ESI)

Exploring the Role of Vacancy Defects on the Optical Properties of $LiMgPO_4$

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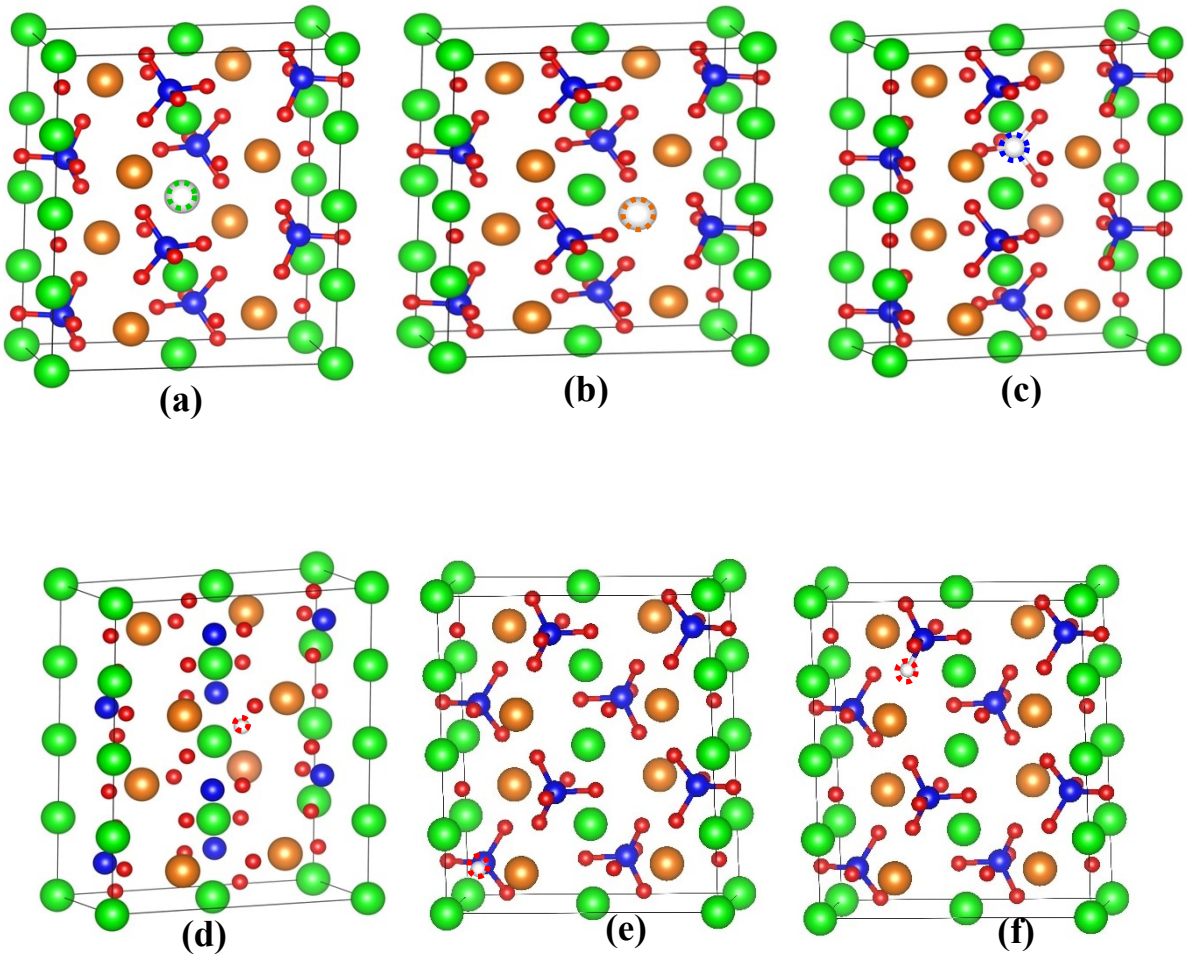

Fig. S1: Crystal Structure of $LiMgPO_4$ with (a) V_{Li}^0, (b) V_{Mg}^0, (c) V_P^0, (d) V_{O1}^0, (e) V_{O2}^0, and (f) V_{O3}^0.

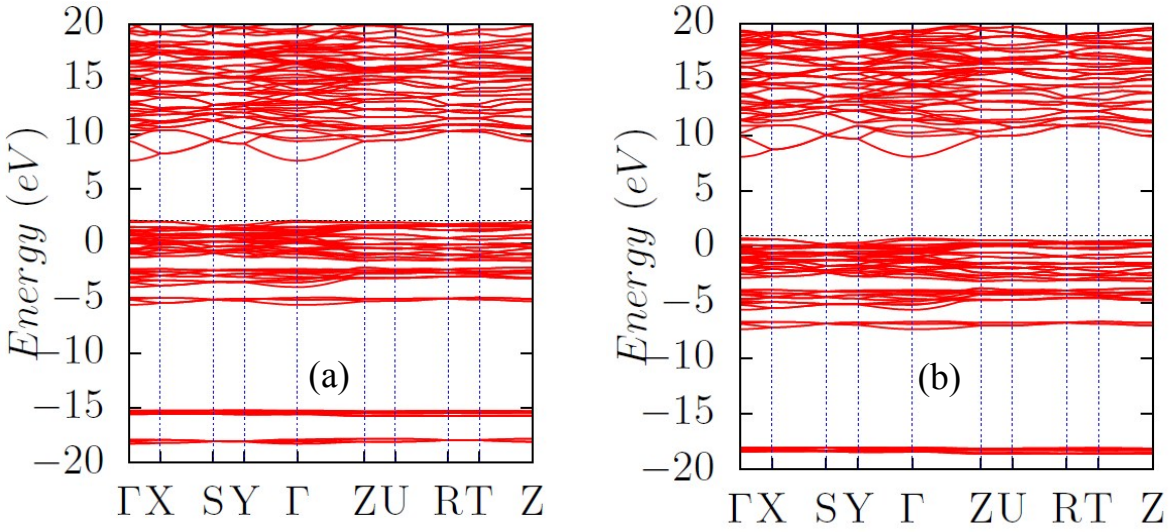

Fig. S2: Band structure of $LiMgPO_4$ using different exchange correlation functionals (a) PBE, (b) HSE06. Horizontal dashed lines indicate Fermi level.

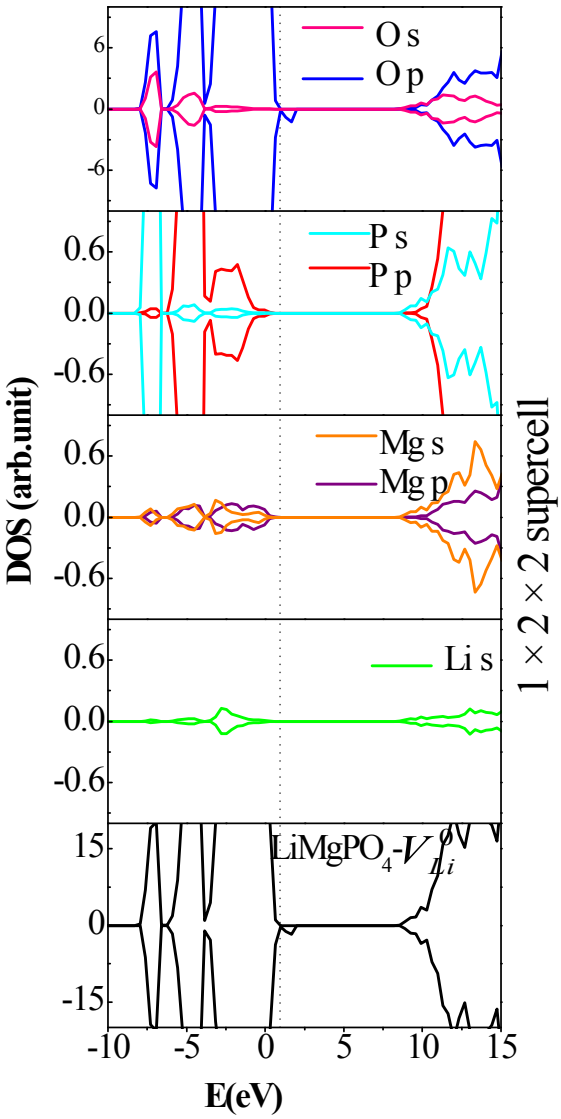

Fig. S3: Density of states of $LiMgPO_4$ containing one neutral Li vacancy using 1 × 2 ×2 supercell. Vertical dashed lines indicate Fermi level.

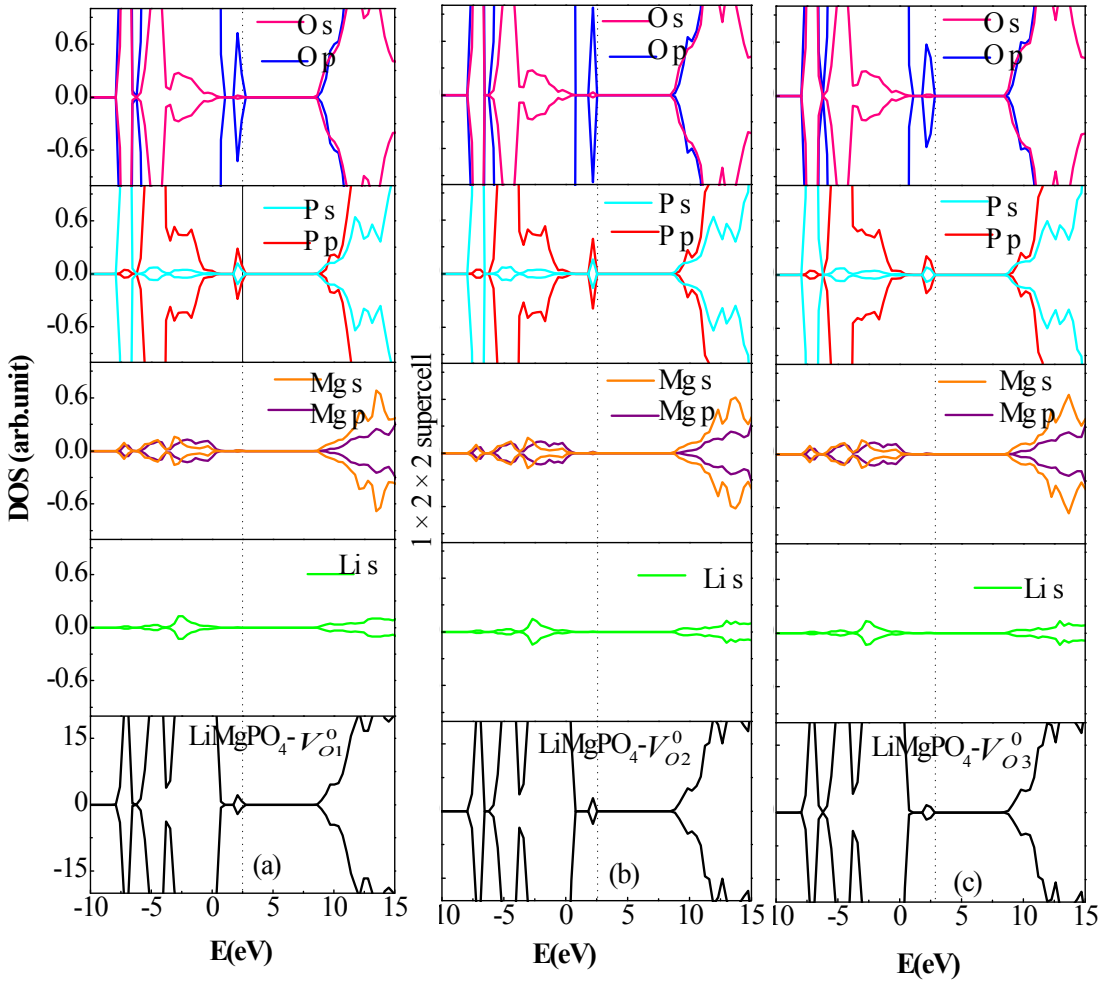

Fig. S4: Density of states of $LiMgPO_4$ containing one neutral O vacancy at (a) O1 lattice site (b) O2 lattice site and (c) O3 lattice site using 1 × 2 ×2 supercell. Vertical dashed lines indicate Fermi level.