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First-principles studies of Mg-doped $LiFePO_4$ for lithium ion batteries[1] SIQI SHI, HUA ZHANG, Department of Physics, Zhejiang Sci-Tech University, Hangzhou 310018, China, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68182, USA, AIFANG LIU, KHOON-CHENG LIM, Pleiades Battery Manufacturing Co., Ltd, Suzhou 215123, China — We investigate the formation energy, crystal parameters and electronic properties of Mg-doped (Li site and Fe site) lithium iron orthophosphate ($LiFePO_4$) by using the first-principles calculations. We noticed that the Mg ions are much more easier to be doped on Fe site than Li site. Comparing with the pure $LiFePO_4$, we found the band gap of Mg-doped $LiFePO_4$ is a little narrower than that of the pure one, indicating that the enhancement of the electronic conductivity upon doping is likely. Furthermore, we discovered that Mg doped on the Fe site causes the bond length to change, which is consistent with our experimental data. The reduction of the Mg-O bond length favors the formation of Li^+ diffusion channels, hence improves the ionic dynamic properties of the olivine $LiFePO_4$. Mg-doped $LiFePO_4$ has bigger electricity peak area that the pure one, which is an indication of improved ionic diffusion.

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