Short Communication

Effect of Antisite Defects on Li Ion Diffusion in LiNiPO₄: a First Principles Study

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Lithium diffusion properties in crystalline LiNiPO₄ were studied using density functional theory. Formation and clustering energies of Li-Ni antisite defects are calculated, results showed the antisite defects are energetically favorable in the LiNiPO₄ and they not tend to bind together. The energy barrier of Li is 0.28 eV in the pristine LiNiPO₄. The energy barriers of Li diffusion along the [010] direction in the LiNiPO₄ were not affected so much compared with that in the pristine system, however, the diffusion energy barrier of Ni diffusion was much larger than that of Li. This indicates that the existence of antisite defect will severely impede Li diffusion along the [010] direction and thus explains the poor cycling performance of LiNiPO₄ cathode materials for LIBs.

Keywords: Li ion batteries, DFT, antisite defects, cathode, LiNiPO₄

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