Effect of Zn-Incorporation into $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ Solid Electrolyte on Structural Stability and Electrical Conductivity: First-Principles Study

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The electronic structures of Zn doped tetragonal $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ at different locations are studied by using the first principles method based on DFT, and the structure optimization, energy band, density of states and population analysis are carried out. Results show that the mixed system of total energy is reduced, the structure is more stable, and Li doping of total energy of -53104eV, more stability. Due to the effect of electrons in different orbitals of Zn, the band number near Fermi level increases, the band gap decreases, the energy required for electron or hole transition decreases, and the conductivity increases. The band gap of La site doping is 3eV, and the conductivity is relatively high. Population analysis proves that the Zn-O bond length of the $\text{Li}_6\text{ZnLa}_3\text{Zr}_2\text{O}_{12}$ system is 1.947Å, which is shorter than the $\text{Li}_7\text{La}_2\text{ZnZr}_2\text{O}_{12}$ system and has better stability. In addition, the length of the Li-Li bond in the doped system is shortened, and the Coulomb repulsion force between Li^+ and Li^+ is increased, which is conducive to increasing the concentration of Li vacancies, thereby improving the conductivity. Although doping can improve stability and conductivity, the amount of doping is too large, which is not conducive to improving the conductivity.

Keywords: $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$, Zn-incorporation, Electronic structure, First-principles

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