

## Study on Electrical Structure and Conductivity of Ti Doped LiFePO<sub>4</sub>

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**1. Introduction:** LiFePO<sub>4</sub> and doped LiFePO<sub>4</sub> is known as electrode material for Li ion batteries because of high Li capacity. In this study, we predicted the electric conductivity of LiFePO<sub>4</sub> and Ti doped LiFePO<sub>4</sub> based on tight-binding calculation.

**2. Methods:** We optimized the structure of calculation model by using density functional theory calculation. Then we calculate the electrical structure of the LiFePO<sub>4</sub> model by original tight binding quantum chemistry calculation code “New-Colors”, and estimated the electric conductivity by “Colors-Cond”.

**3. Results and Discussion:** Figure 1 shows the calculation model of Ti-doped LiFePO<sub>4</sub>. Figure 2 shows the partial density of states (PDOS). An impurity level derived from Ti 3d appeared between the top of valence and bottom of conduction band. Table 1 shows the estimated and measured electric conductivity.[1] The estimated electric conductivity of pure LiFePO<sub>4</sub> agreed with the experimental data. Compared with pure LiFePO<sub>4</sub>, Ti-doped LiFePO<sub>4</sub> has higher electric conductivity.

### References

[1] HU Guo-rong, Trans. Nonferrous Met. SOC . China 17(2007) 296-300.

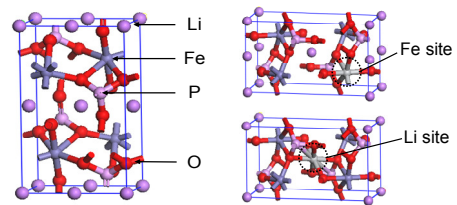


Fig.1 simulation model

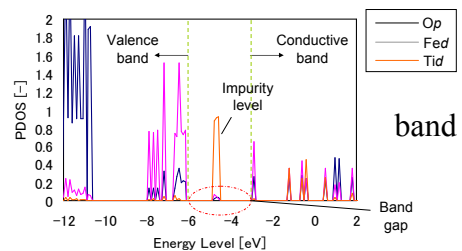
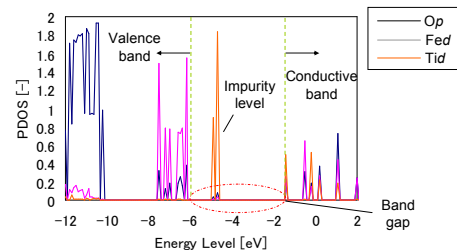


Fig.2 PDOS (1) Fe site doped LiFePO<sub>4</sub>  
(2) Li site doped LiFePO<sub>4</sub>

Table 1 Electrical Conductivity Calculation Result

Model	Calc. (S/cm)	Expt. (S/cm)
LiFePO <sub>4</sub>	$3.32 \times 10^{-8}$	$10^{-3}$ [1]
Ti doped (Li site)	$1.62 \times 10^{-1}$	—
Ti doped (Fe site)	$8.89 \times 10^{-4}$	—