Ferroelectric Polarization in Poly(vinylidene difluoride) by DFT calculation

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Poly(vinylidene difluoride) (PVDF) polymer has been well used for binder materials in lithium-ion batteries (LIB). However, effects of crystalline phase of the PVDF on LIB were rarely demonstrated. Here, the electronic properties and lithium ion affinity of paraelectric α phase PVDF and ferroelectric β phase PVDF were investigated using density functional theory calculations. A strong polarization of the ferroelectric β phase PVDF leaded to surface metallization by shifting local bands in electronic density of states. More specifically, the polarization increased an amount of charge transfer significantly between each polymer layer and varied the work functions to a large extent (i.e. 8.3 eV for F-terminated surface and 1.6 eV for H-terminated surface), which was expected to play a crucial role in reducing charge transfer resistance. Furthermore, the ferroelectric polarization enhanced the binding affinity of lithium ion, which resulted in the promotion of lithium ions accessing toward the electrode surface. To this end, we found that ferroelectric polarization of PVDF is good to facilitate charge transfer and lithium ion diffusion in the vicinity of active electrodes.