Prediction of properties of organic ferroelectrics and piezoelectrics by first-principles calculation

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Organic ferroelectrics and piezoelectrics are promising materials since they contain neither toxic nor rare elements. Recently, we observed the transition from an antiferroelectric (AFE) phase to a ferroelectric (FE) phase under a strong electric field on squaric acid (SQA) and proposed two possible FE phases (FE-α and FE-β) with their molecular arrangements and space groups [1]. The experimentally observed FE phase is thought to be the FE-α phase. On the other hand, the FE-β phase has not yet been experimentally confirmed.

In the present study, by computationally applying a static electric field [2], we simulate the AFE-to-FE transitions in SQA [3]. The calculations are performed using the computational code QMAS. As for the exchange-correlation functional, to reproduce the lattice parameters accurately, the rVV10 functional [4] is used.

Depending on the direction of the electric field, two different metastable ferroelectric (and piezoelectric) phases have been found. One of them corresponds to the experimentally confirmed FE-α phase, whereas the other corresponds to the FE-β phase. The spontaneous polarization values of the phases are 14.5 and 20.5 μC/cm^2, respectively. They are relatively high among those of the existing organic ferroelectrics. Their crystal structures are obtained as a function of the electric field. Significant converse piezoelectric effects are observed for both the phases as shown in Fig. 1 ($\sim$10 pm/V).

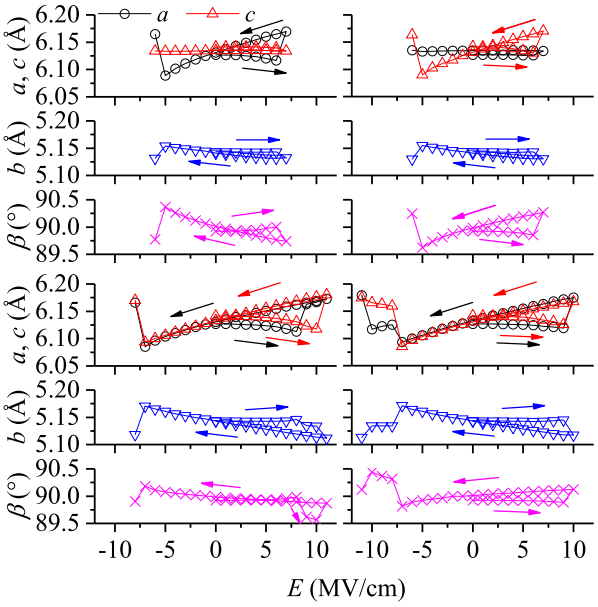

Figure 1: Variation in lattice parameters under electric field. $\boldsymbol{E} \parallel$ (upper left) $\boldsymbol{x}$, (upper right) $\boldsymbol{z}$, (lower left) $\boldsymbol{x}+\boldsymbol{z}$, and (lower right) $\boldsymbol{x}-\boldsymbol{z}$.

References

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