

Spontaneous Self-formation of Molecular Ferroelectric Heterostructures

Kaige Gao^{a*}, Zhen Su^a, Chen Li^b, , Di Wu^b Binbin Zhang^c

^aCollege of Physical Science and Technology, Yangzhou University, Jiangsu 225009, P. R. China

^bDepartment of Materials Science and Engineering, College of Engineering and Applied Sciences, Nanjing University, Nanjing 210093, P. R. China.

^cState Key Laboratory of Solidification Processing & Key Laboratory of Radiation Detection Materials and Devices & School of Materials Science and Engineering, Northwestern Polytechnical University, Xi'an 710072, P. R. China.



Fig. S1. Digital photo of the obtained DIPAP microrods sample in a PTFE mold.

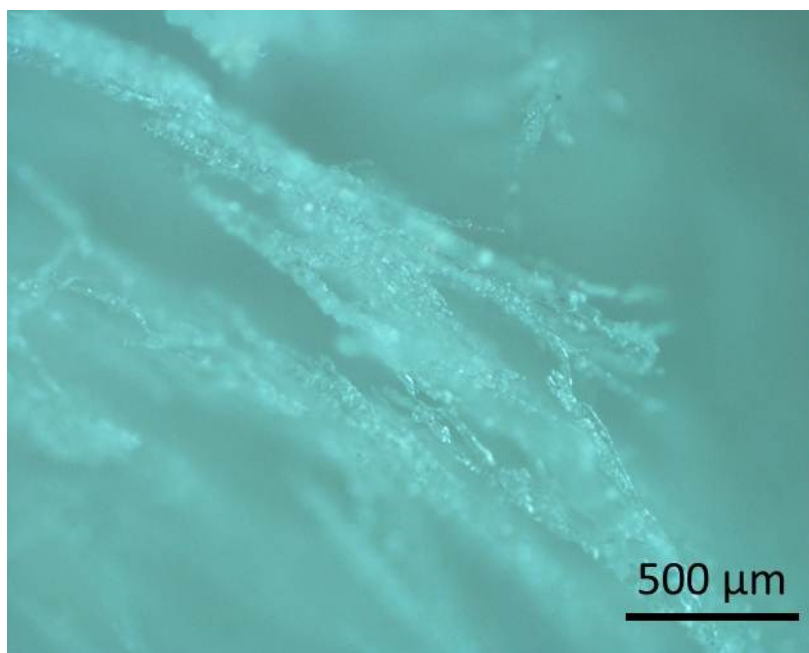


Fig. S2. Microscopic photograph of the obtained DIPAP microrods.

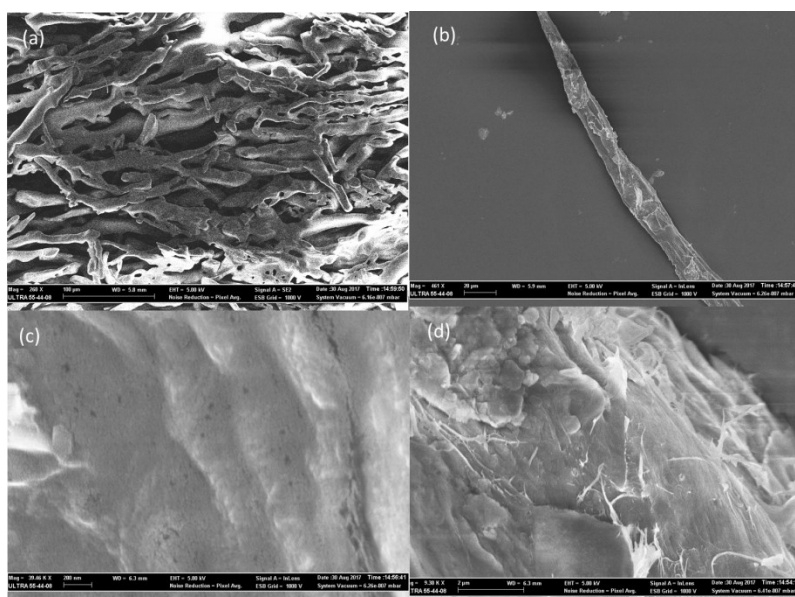


Fig. S3. SEM of DIPAP micron rods.

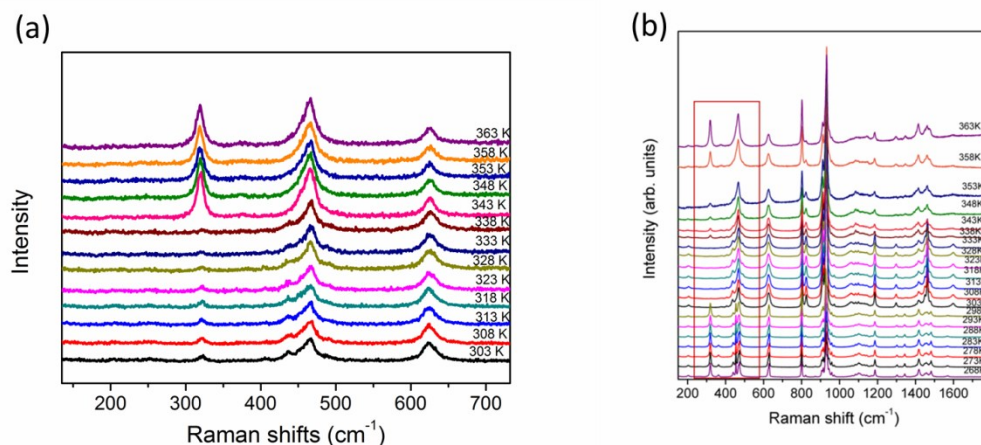


Fig. S4. (a) Variable-temperature Raman spectra of DIPAP single crystals with (a) non-zero and (b) almost zero peak intensity at 319 cm⁻¹ at room temperature.

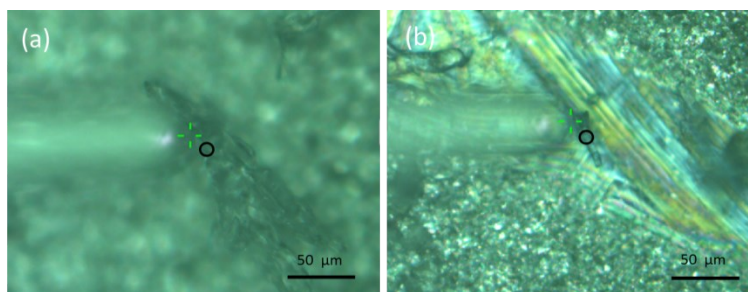


Fig. S5. Optical microscope images of (a) thick and (b) thin DIPAP microrods during the PFM measurements. Figs. 2a and 2b were measured at the black circle in Fig. S5(a). Figs. 2c and 2d were measured at the black circle in Fig. S5(b).

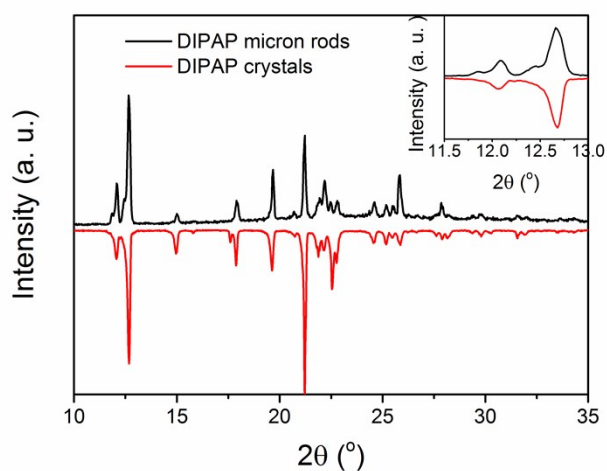


Fig. S6. Comparison of the PXRD patterns of DIPAP microrods and DIPAP crystals.

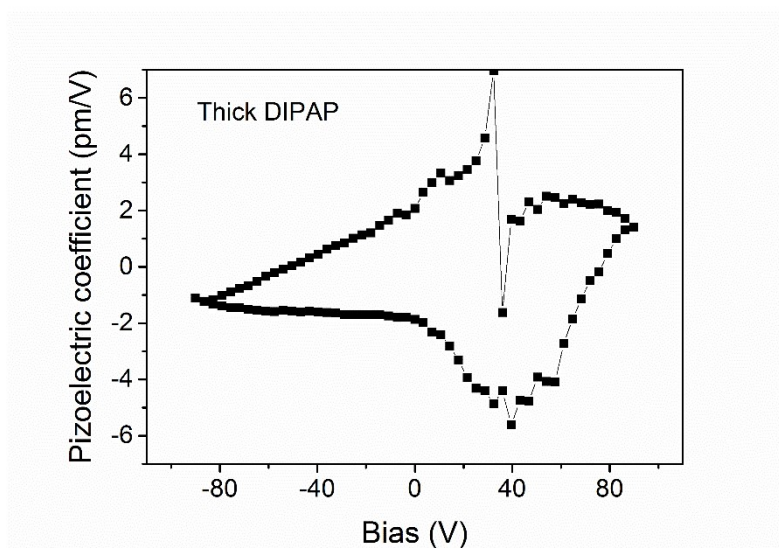


Fig. S7. Piezoelectric coefficient of thick DIPAP microrods derived from the PFM amplitude hysteresis loop in Fig. 2c.

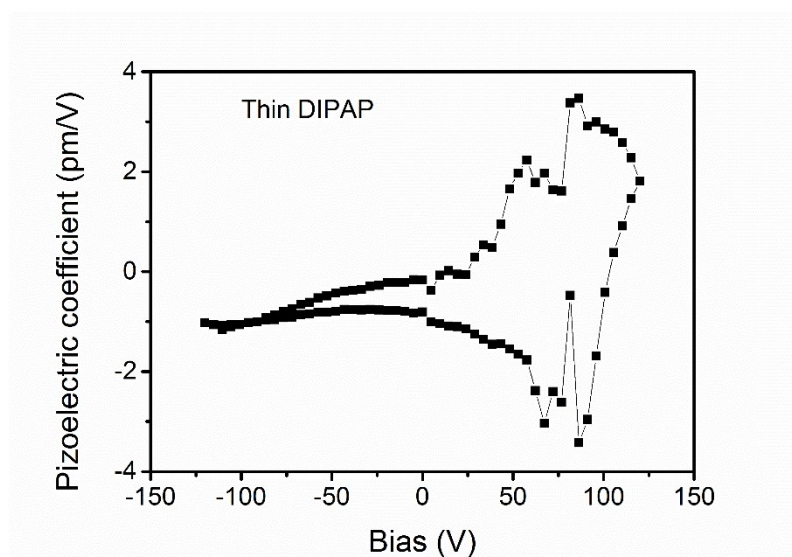


Fig. S8. Piezoelectric coefficient of thin DIPAP microrods derived from the PFM amplitude hysteresis loop in Fig. 2d.

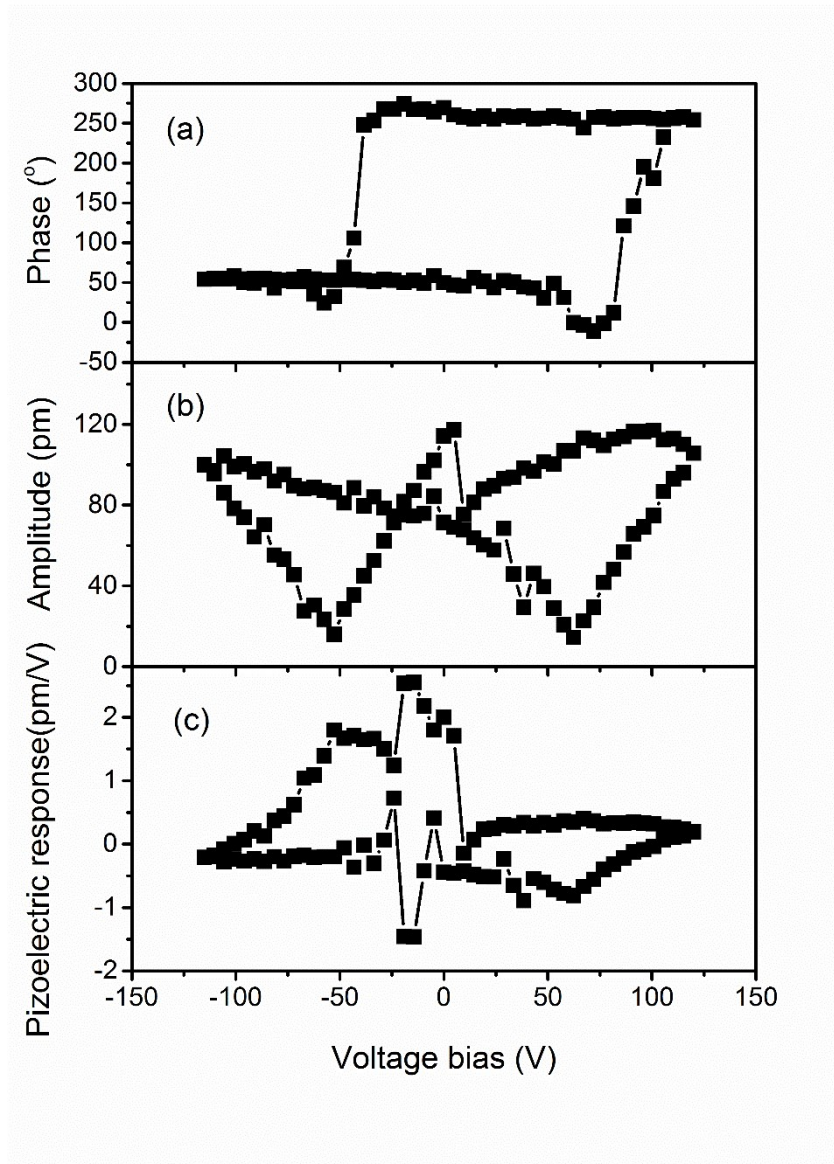


Fig. S9. (a) PFM phase and (b) amplitude hysteresis loops measured for a DIPAP single crystal. (c) Piezoelectric coefficient of a thick DIPAP single crystal derived from (b).

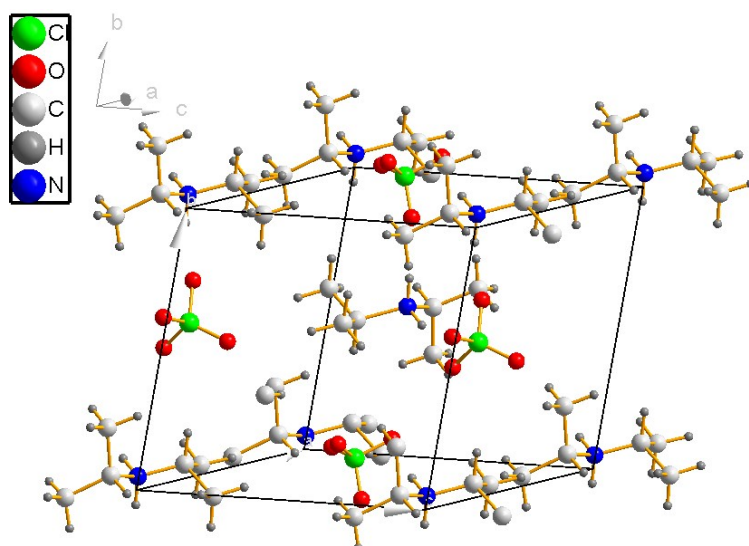


Fig. S10 Crystal structure of DIPAP at room temperature. The space group is $P1$, $a=8.15 \text{ \AA}$, $b=8.52 \text{ \AA}$, $c=8.77 \text{ \AA}$, $\alpha=82.77^\circ$, $\beta=65.14^\circ$, $\gamma=79.9^\circ$.

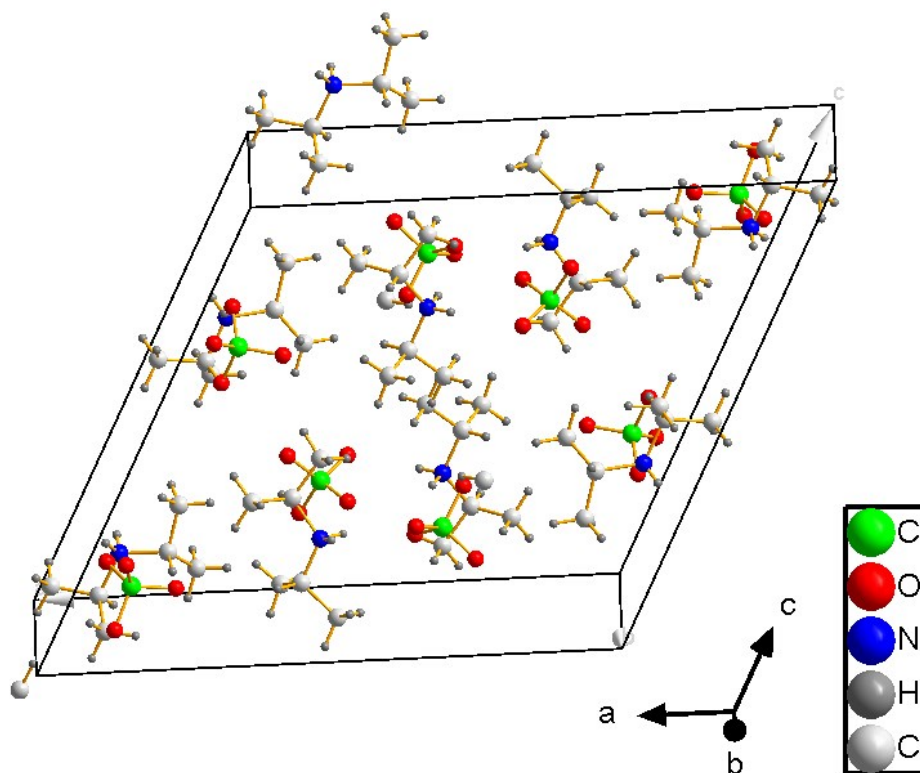


Fig. S11 Crystal structure of DIPAP at 263 K. The space group is $P2_1/c$, $a=17.70 \text{ \AA}$, $b=8.25 \text{ \AA}$, $c=16.06 \text{ \AA}$, $\alpha=90^\circ$, $\beta=116.33^\circ$, $\gamma=90^\circ$.

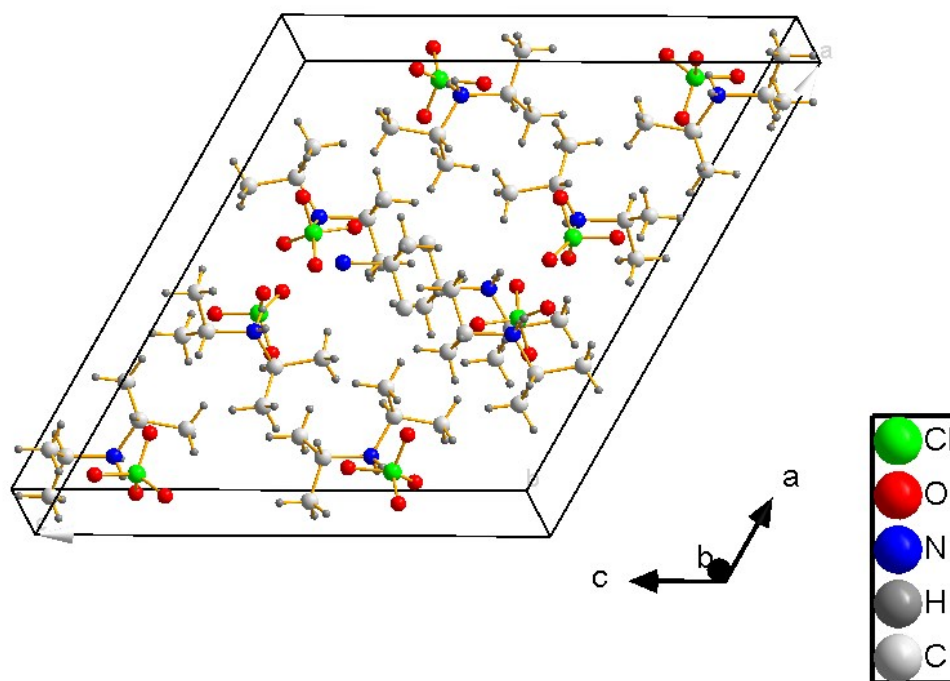


Fig. S12 Crystal structure of DIPAP at 383 K. The space group is $P2_1/c$, $a=17.66 \text{ \AA}$, $b=8.79 \text{ \AA}$, $c=16.67 \text{ \AA}$, $\alpha=90^\circ$, $\beta=118.59^\circ$, $\gamma=90^\circ$.

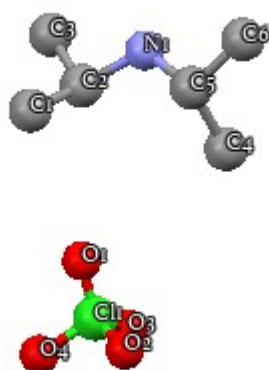


Fig. 13 Molecule structure of DIPAP. The hydrogen atoms was erased.