Supporting Information for: Order-disorder phase transition and orientational defect formation in a hybrid organic-inorganic piezoelectric material

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SUPPORTING FIGURES

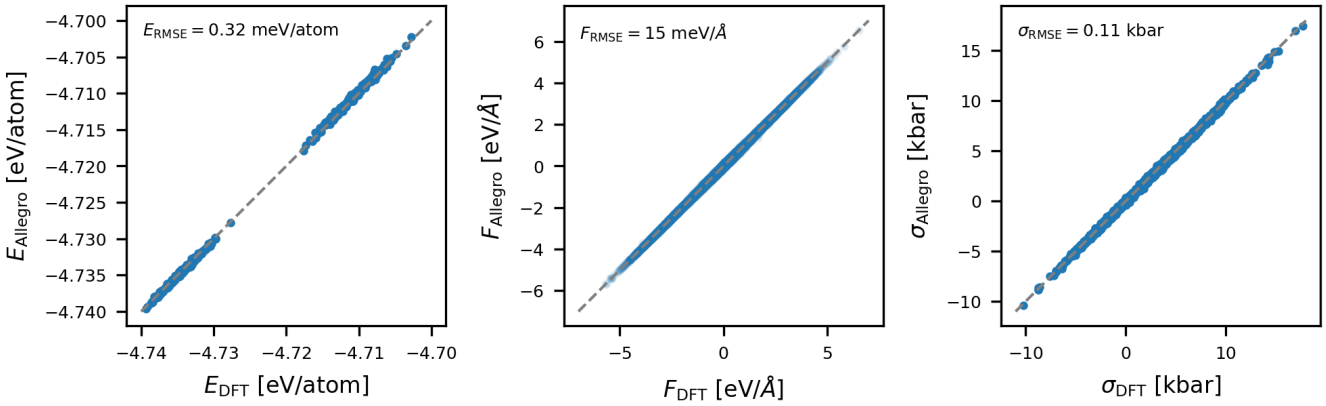

FIG. S1. Parity plot showing the agreement between density functional theory calculation with the PBEsol functional and the trained Allegro machine learning force field for per atom energies, force components and stress components on a hold out test set.

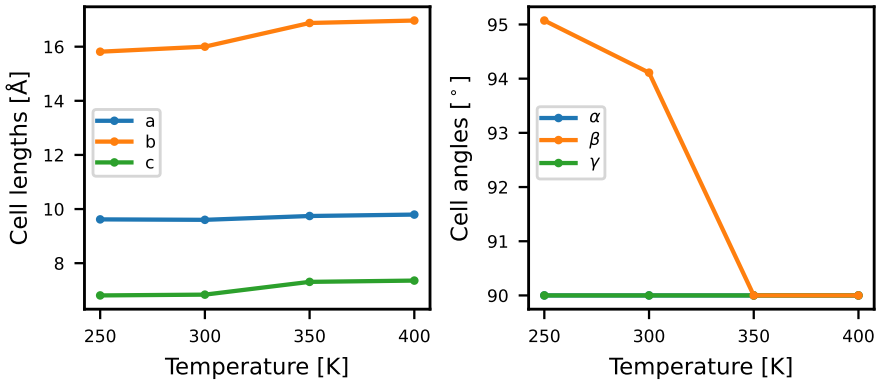

FIG. S2. Cell parameters (unit cell lengths and angles) from MLFF MD simulations in the NPT ensemble for the trained Allegro MLFF without inclusion of dispersion interactions. The phase transition temperature is significantly underestimated. The agreement with experiment is improved by inclusion of dispersion interaction as seen in Figure 2 in the main text.

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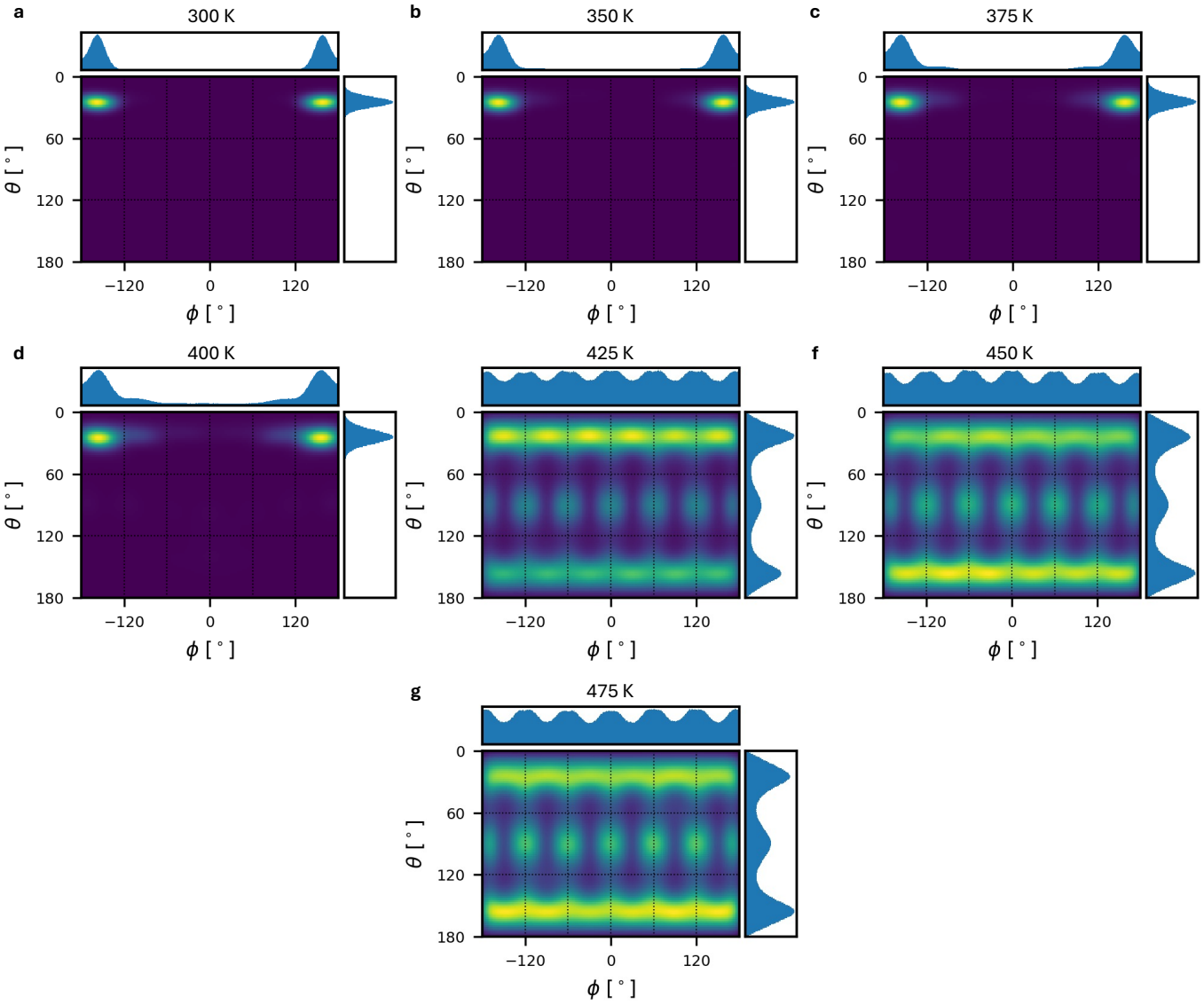

FIG. S3. Density map of orientations of TMCM dipolar cations **a** 300 K, **b** 350 K, **b** 375 K, **d** 400 K, **e** 425 K, **f** 450 K, and **g** 475 K.