Supplementary material

Achieving Excellent High-Temperature Energy Storage Performance in Aromatic Polymer Films via Multi-Scale Interface Engineering

Tianyuan Yin[#2], Ying Chen[#2], Yue Zhang[23], Chao Yin[23], Xue Hongbo[2], Tiandong Zhang[123]*

1 National Key Laboratory of High-performance Special Cable Technology, Harbin 150080, PR China

2 School of Electrical and Electronic Engineering, Harbin University of Science and Technology, Harbin 150080, PR China

3 Key Laboratory of Engineering Dielectrics and Its Application, Ministry of Education, Harbin University of Science and Technology, Harbin 150080, PR China

[#]Co-first authors: Tianyuan Yin, Ying Chen

*Corresponding author: Tiandong Zhang

E-mail: tdzhang@hrbust.edu.cn

Molecular dynamics simulation: Molecular structure modeling was performed using Materials Studio software, with all models undergoing geometric optimization under the COMPASS II force field. The molecular model was constructed using the Amorphous Cell module, placing 50 molecular chains within a periodic box with a side length of 40 Å. Each chain comprised five repeating units. During the simulation, the long-range potential correction for particle-particle-mesh interactions was set to 10^{-4}, and the temperature was gradually lowered from 800 K to 298 K. When the system reached energy equilibrium at 298 K under standard atmospheric conditions, the resulting structure was used to calculate the free volume and occupied volume.

Weibull distribution of breakdown field strength： The breakdown strength test for composite films is based on the statistical distribution following the Weibull distribution (Formula), with the sample size of 10 per test. E_i denotes the breakdown strength of the i^{th} sample, and E_b corresponds to the characteristic breakdown strength associated with a breakdown probability of 63.2%. β is the shape parameter used to assess the degree of data dispersion, reflecting the stability of the composite film's breakdown strength.

$$P(E) = 1 - \exp[-\left(\frac{E_i}{E_b}\right)^{\beta}]$$

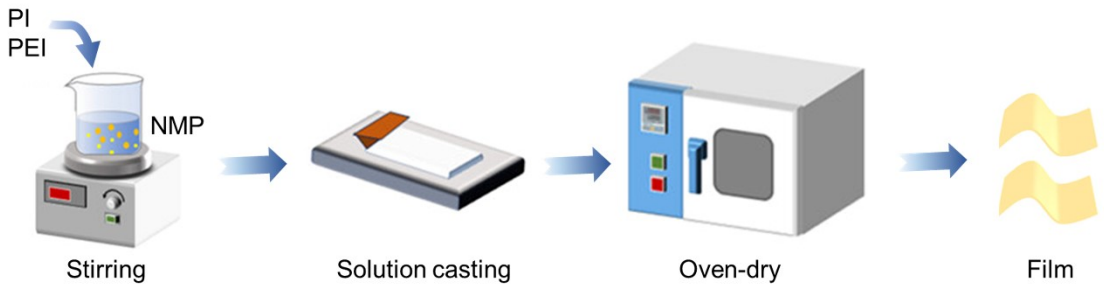

Fig. S1 Schematic diagram of the CNO nanosheet preparation process.

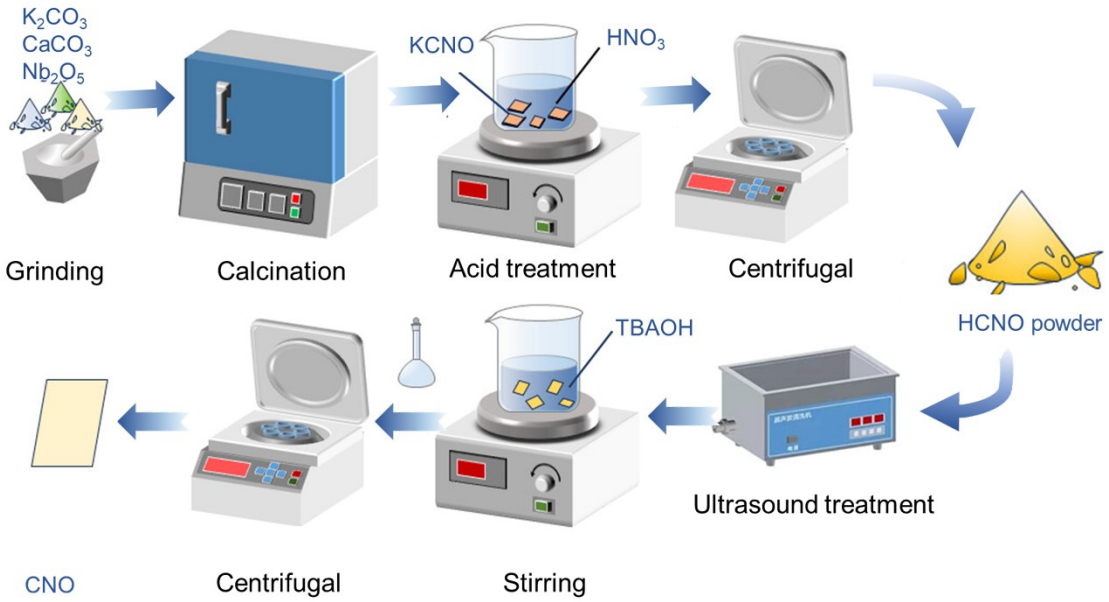

Fig. S2 Schematic diagram of the fabrication process for the composite dielectric film.

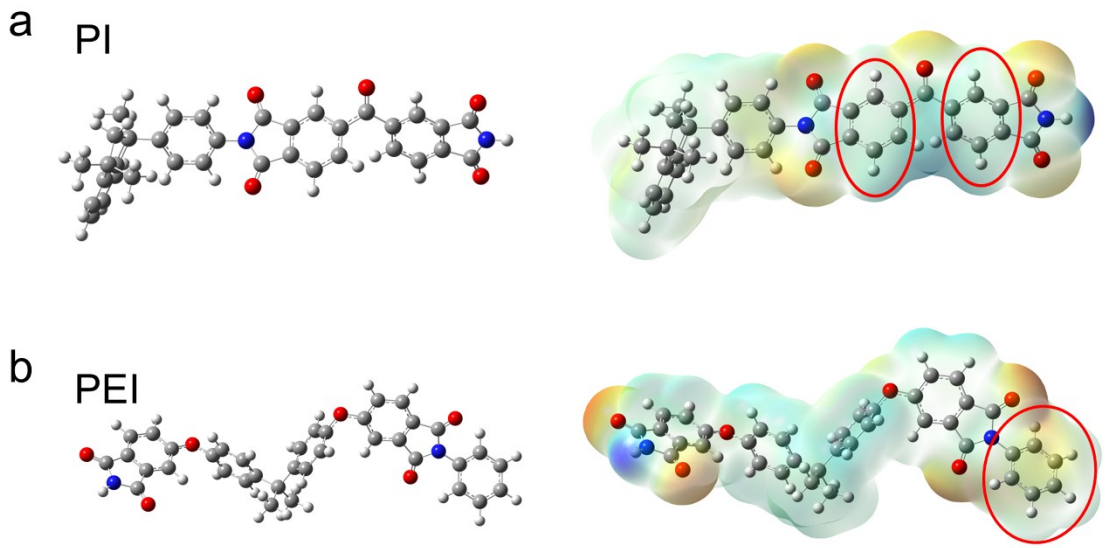

Fig. S3 Schematic chemical structure and electrostatic potential distribution of (a)PI and (b) PEI.

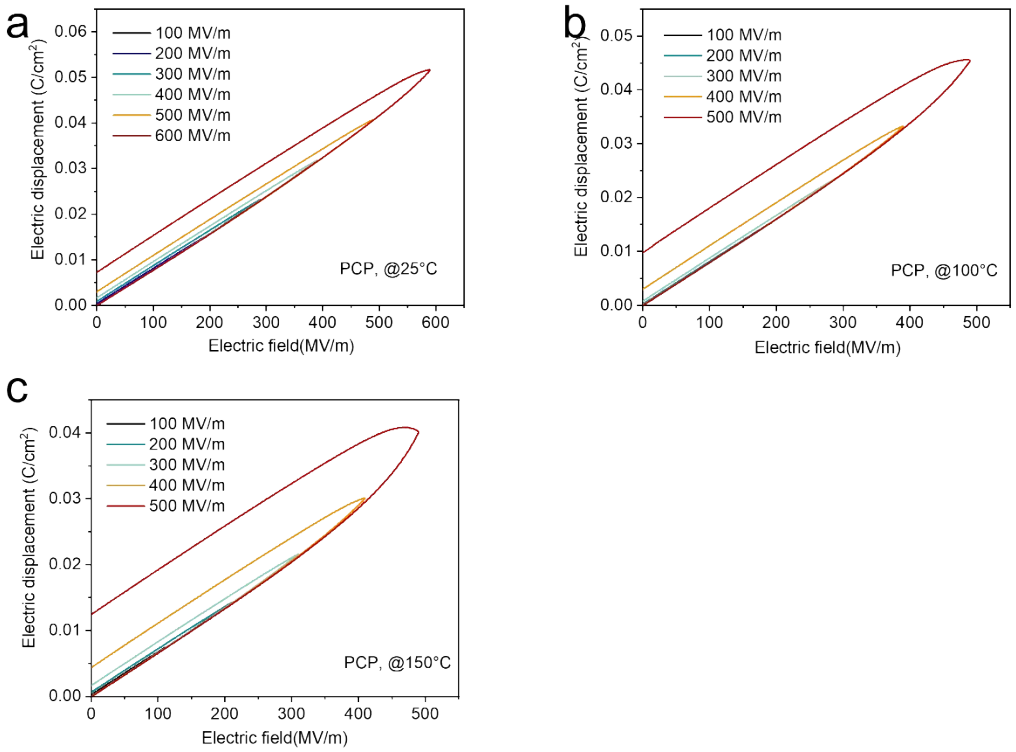

Fig. S4 D-E loops of PCP composite films. (a) 25℃, (b) 100℃, (c) 150℃.

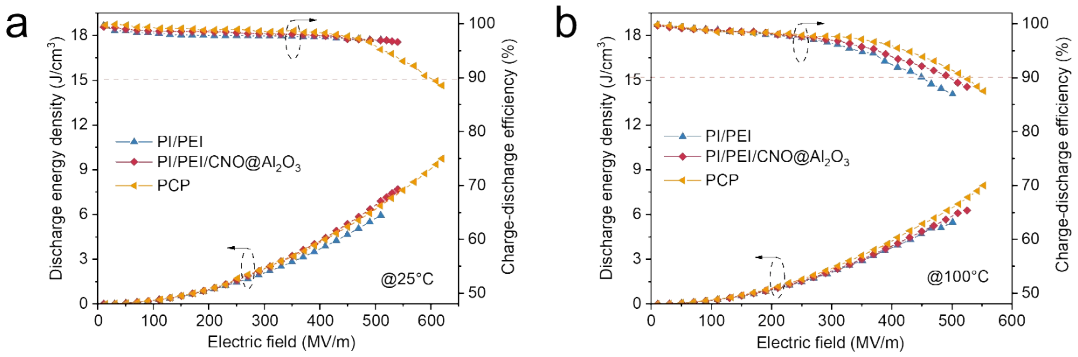

Fig. S5 Energy storage performances of the films at different temperatures. (a) 25℃ and (b) 100℃.

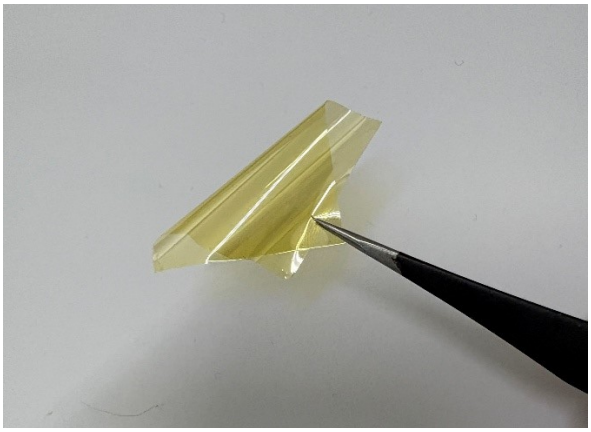

Fig. S6 Bending diagram of PCP composite film.