Electronic Supplementary Material (ESI) for Journal of Materials Chemistry

Supporting information

Targeted Synthesis of an Electroactive Organic Framework

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1. Materials.

The starting materials and solvents were purchased from Aldrich. In electrochemical experiments, tetra-butylammoniumhexafluorophosphate (Bu_4NPF_6), tetra-butylammoniumperchlorate (Bu_4NClO_4), tetra-butylammoniumtetrafluoroborate (Bu_4NBF_4) and tetraethylammonium-toluene-4-sulfonate (ET_4TOS) were electrochemical grade and were obtained from Aldrich.

2. Topology design of 3D Frameworks

The 3D model of JUC-Z2 was obtained with the Materials Studio simulation environment (Version 4.3) employing MS Visualizer. The structures were generated by beginning with the space group *p6/mmm*. Laid the center nitrogen atom of the triphenylamine on the trigon centroid, and replaced the C-N bonds with the phenyl rings. Then we performed energy minimization and geometry optimization calculations employing universal and COMPASS force-field to obtain reasonable structures.

3. Investigation of Structure of JUC-Z2

3-1.FTIR of JUC-Z2

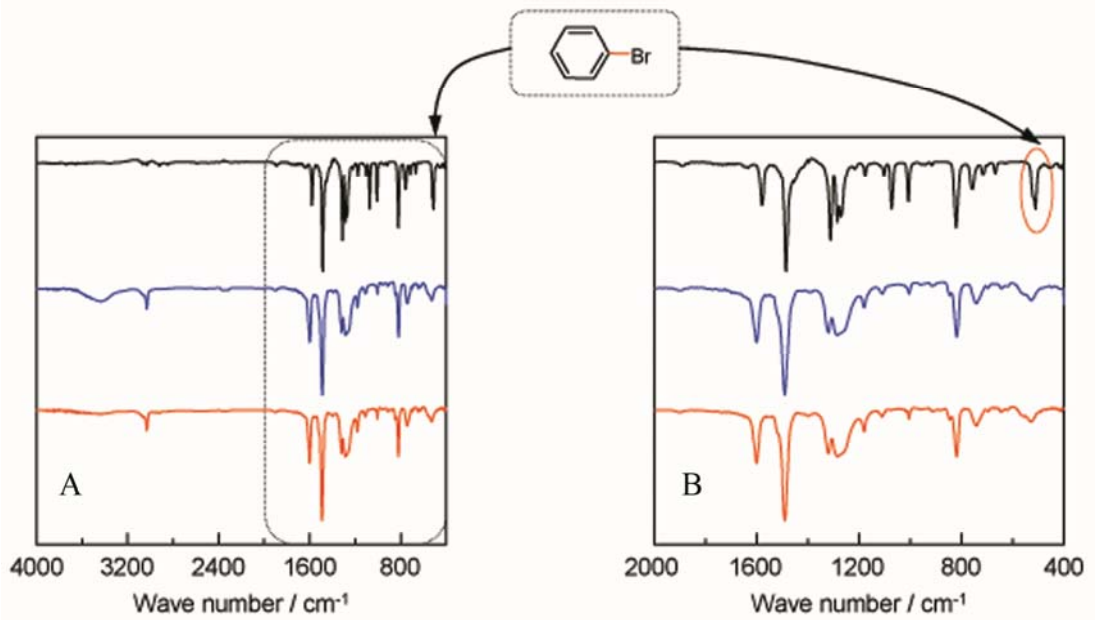

Figure S1. FTIR spectra of the JUC-Z2(red), JUC-Z2-4h (blue) and the TBPN (black) from 400- 4000 cm-1(A) and 400-2000 cm-1 (B). The characteristic adsorption bands for Carbon- Bromine highlighted, clearly showing the lack of bromine in the final product and indicating the formation of the polymeric structure.

3-2. AFM study of Oligo-JUC-Z2 and JUC-Z2

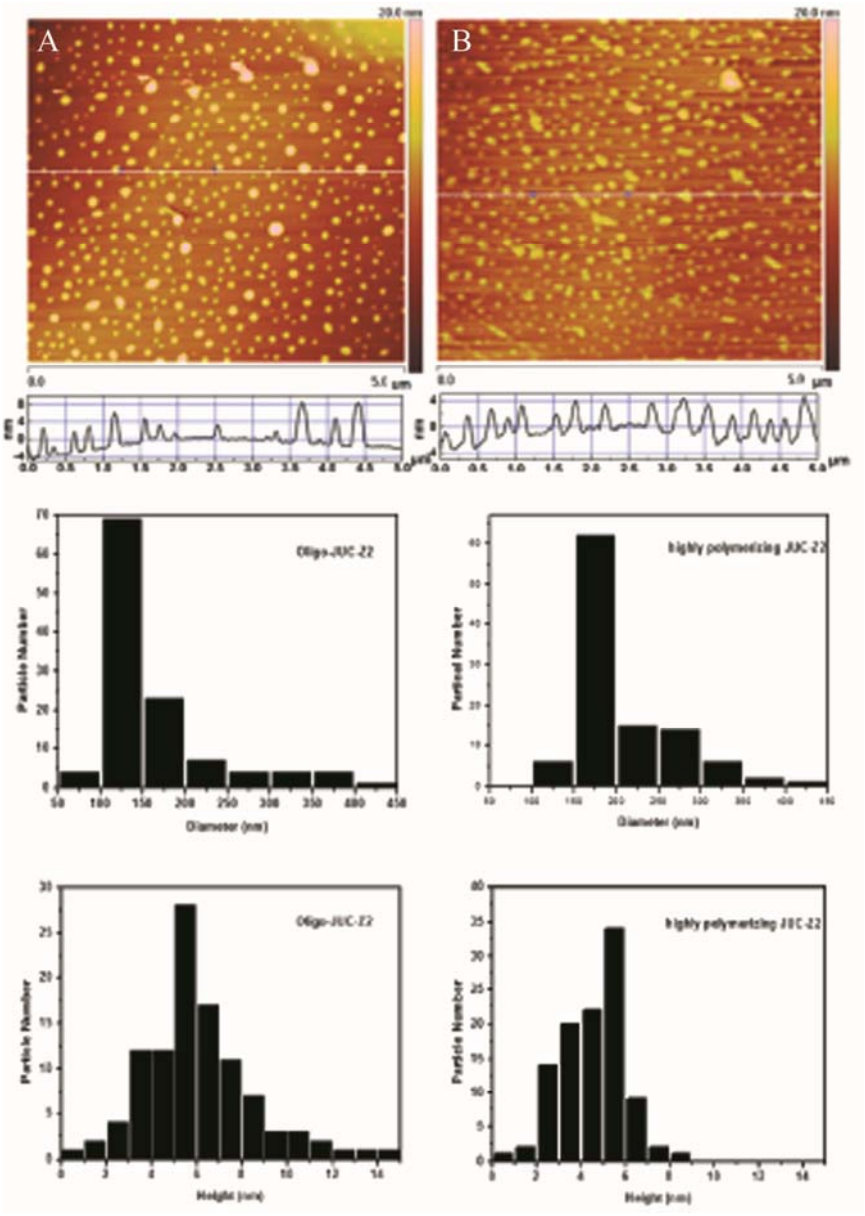

Figure S2. Taping mode AFM images and histogram of Oligo (A) and highly condensed JUC-Z2 (B) on HOPG surface. The white line through the image indicates where the section profile was measured.

3-3. PXRD of JUC-Z2

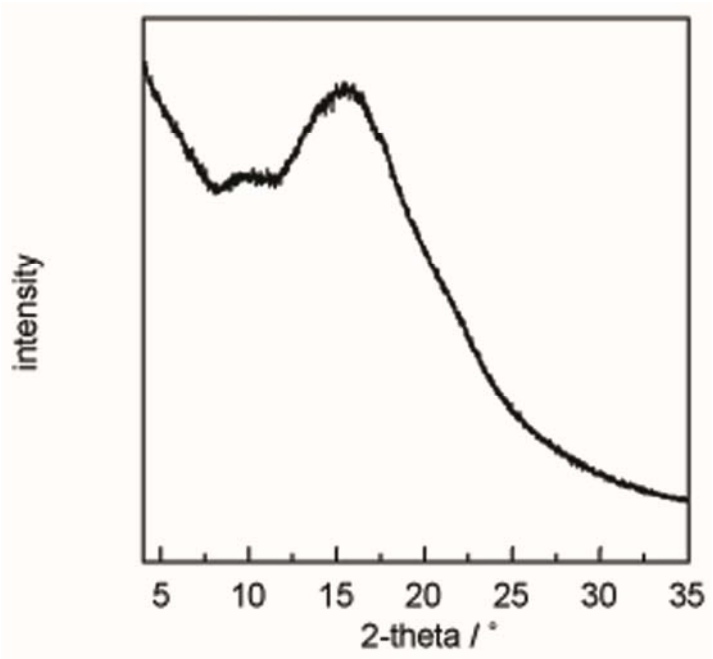

Figure S3 The PXRD pattern of JUC-Z2

4. Investigation of Stability

4-1. TGA of JUC-Z2

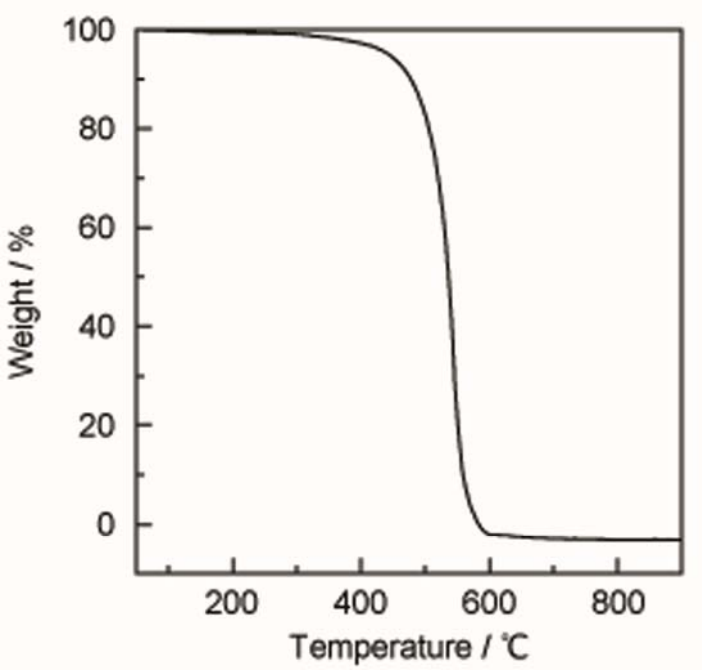

Figure S4. TGA plot of JUC-Z2 at air atmosphere, rate of 10 ^{o}C/ min

5. Investigation of Electrochemical Property

5-1. electrochemical redox process of JUC-Z2

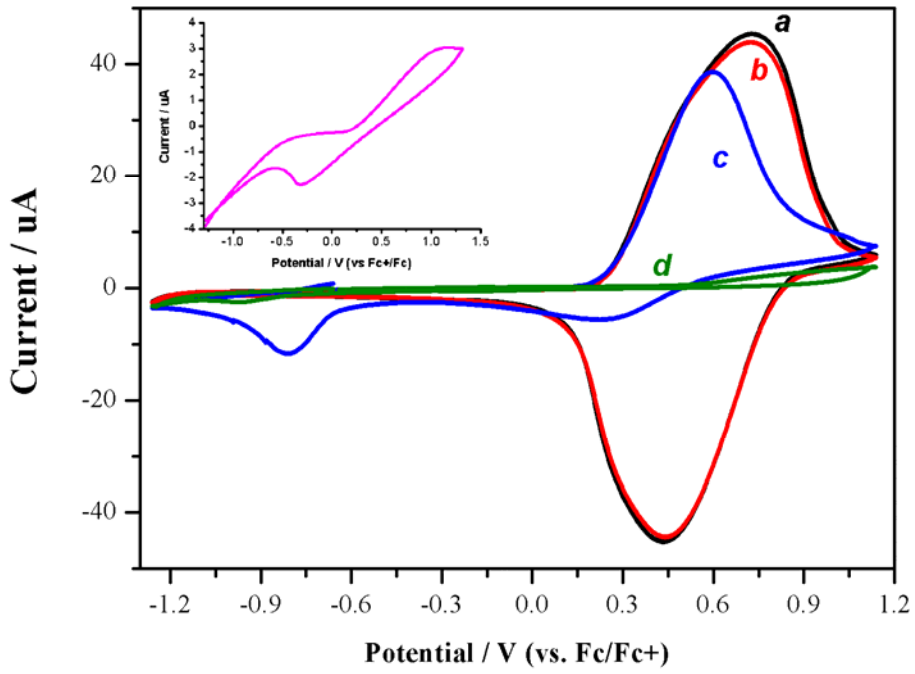

Figure S5. Cyclic voltammogramms of highly condensed JUC-Z2 powder film on Pt microelectrode at a scan rate of 50 mV/s in the degassed acetonitrile solution containing 0.1 M Bu_4NPF_6 at (a) the first and (b) 5th cycle; 0.1 M ET_4TOS at (c) the first and (d) 5th cycle; (inset) 0.1 M CSA at the first cycle.

6. References

[1] C. S. Cha, C. M. Li, H. X. Yang, P. F. Liu, *J. Electroanal. Chem*. **1994**, *368*, 47.

[2] J. K. Feng, Y. L. Cao, X. P. Ai, H. X. Yang, *J. Power Sources* **2008**, *177*, 199.