Electronic Supplementary Information

Dibenzo[b,d]furan and Dibenzo[b,d]thiophene Molecular Dimers as Hole Blocking Materials for High-Efficiency and Long-Lived Blue Phosphorescent Organic Light-Emitting Diodes

Seokhoon Jang,^a Kyung Hyung Lee,^b Jun Yeob Lee,^{*b} and Youngu Lee^{*a}

^a Department of Energy Science & Engineering, DGIST, 333, Techno Jungang-daero, Hyeonpung-eup, Dalseong-gun, Daegu, 42988, Republic of Korea. E-mail: <u>youngulee@dgist.ac.kr</u>; Tel: +82-53-785-6414; Fax: +82-53-785-6409.

^b School of Chemical Engineering, Sungkyunkwan University, 2066, Seobu-ro, Jangan-gu, Suwon-si, Gyeonggi-do, 16419, Republic of Korea.
E-mail: <u>leej17@skku.edu</u>.



Fig. S1 ¹H NMR spectrum of compound 1'.

6-Bromo-2-iododibenzo[b,d]thiophene (compound 1')_C NMR



Fig. S2 ¹³C NMR spectrum of compound 1'.



Fig. S3 ¹H NMR spectrum of compound 2.



Fig. S4 ¹H NMR spectrum of compound 3.



Fig. S5¹³C NMR spectrum of compound 3.

DBF-d-PO_H NMR



Fig. S6 ¹H NMR spectrum of DBF-d-PO.



Fig. S7 ¹H NMR spectrum of DBT-d-PO.

DBF-d-Py_H NMR



Fig. S8 ¹H NMR spectrum of DBF-d-Py.



Fig. S9 ¹³C NMR spectrum of DBF-d-Py.



Fig. S10 ¹H NMR spectrum of DBT-d-Py.



Fig. S11 ¹³C NMR spectrum of DBT-d-Py.



Fig. S12 (a, b) DSC traces of DBF-d-PO and DBT-d-PO and (c, d) DTA traces of DBF-d-Py and DBT-d-Py.



Fig. S13 AFM topographic images of DBF-d-PO, DBT-d-PO, DBF-d-Py, and DBT-d-Py before thermal annealing treatment.



Fig. S14 AFM topographic images of DBF-d-PO, DBT-d-PO, DBF-d-Py, and DBT-d-Py after thermal annealing treatment (85 °C, 24 h).



Fig. S15 UV-vis absorption spectra of DBF-d-PO, DBT-d-PO, DBF-d-Py, and DBT-d-Py in film.



Fig. S16 Reduction traces of DBF-d-PO, DBT-d-PO, DBF-d-Py, and DBT-d-Py in CV.