Diimide nanoclusters play efficient electron injection/transport role in organic light-emitting devices

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Figure S1. Shape change of energy minimized 3D structure of Bphen-BCDI by rotation according to the vertical axis.

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Figure S2. DSC thermogram of Bphen-BCDI, which is extended up to 375 °C: No melting point is observed in this range.



Figure S3. UV-visible absorption spectrum of Bphen-BCDI film on quartz substrate: No ground state charge transfer complexes are observed.



Figure S4. Cross-sectional structure of OLED fabricated in this work: Each molecular structure is also shown here.



Figure S5. Current efficiency (η_c) of OLED as a function of current density (J).



Figure S6. Luminance of OLED as a function of current density (J).



Figure S7. Auger electron spectra of each atom as a function of kinetic energy for the sample [glass/ITO/HIL/HTL/EML/BAlq]: The atomic composition was measured at two different points (see the

inset table).



Glass/ITO/HIL/HTL/EML/HBL(BAIq)/Bphen-BCDI(0.5nm)

Figure S8. Auger electron spectra of each atom as a function of kinetic energy for the sample [glass/ITO/HIL/HTL/EML/BAlq/BPhen-BCDI(0.5nm)]: The atomic composition was measured at two different points (see the inset table).



Figure S9. 3D AFM images: (a) glass/ITO/HIL/HTL/EML/BAlq, (b) glass/ITO/HIL/HTL/EML/BAlq/Bphen-BCDI(0.5nm): The surface roughness (Rg) was calculated using the whole scanned area.



Figure S10. FT-IR spectrum of Bphen-BCDI powder mixed with KBr.



Figure S11. MALDI-TOF-MASS spectrum of Bphen-BCDI powder: The major peak was observed at 602.719 m/z. Other minor peaks can be attributed to the fragmentations and/or clusters made between matrix and product molecules during measurement.



Figure S12. Simulated ¹³C-FT-NMR spectra of PTA (top panel), BCDA (middle panel), and Bphen-BCDI (bottom panel). Note that both the carbon linked with the amine group of PTA and the carbon in the anhydride ring of BCDA exhibited slight chemical shift changes in the BPhen-BCDI owing to the change of their bonding environments.



Figure S13. ¹³C-FT-NMR spectrum of Bphen-BCDI powder: 'a' and 'b' denote the peaks corresponded to the carbon atoms of which bonding environments are changed from their original values in starting materials (PTA and BCDA) as noted in the simulated spectra in Figure S12.