Supplementary Information

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Figure S1: Optimized structures of pyromellitic diimide derivatives (a) BP\(\text{yDI}\) (b) BP\(\text{yDI1}\) (c) BP\(\text{T}\) (d) BP\(\text{PTTF}\) and (e) BPP\(\text{yDI}\).

Figure S2: The change of bond length as a function of bond index of pyromellitic diimide derivatives; (a) oxidation (b) reduction.
Figure S3: Hirshfeld Surface of the pyromellitic diimide derivatives; (a) BPyDI (b) BPyDI1 (c) BPIT (d) BBBIT and (e) BPPyDI.