

Supporting Information

Ambipolar charge-transport property for the D-A complex with naphthalene diimide motif

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1. TGA analysis of 4NH₂-NDI

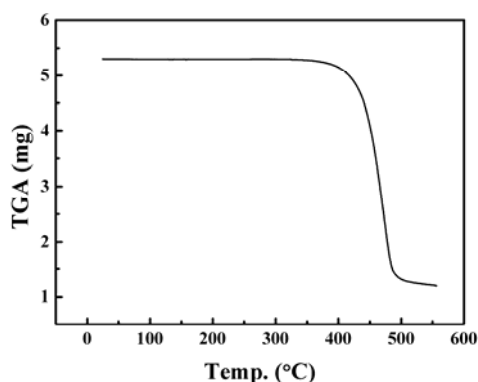


Fig. S1 TGA curves of 4NH₂-NDI from 25 °C to 550 °C with heating rate of 10 °C/min. under nitrogen atmosphere.

2. Absorption spectra of blend thin films of DHNDI and 4NH₂-NDI

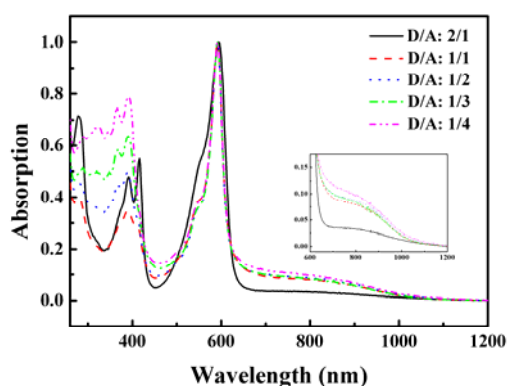


Fig. S2 The absorption spectra of blend thin films of DHNDI and 4NH₂-NDI in different molar ratios.

3. DFT calculation data

Calculation data for 4NH₂-NDI:

| | | Coordinates(Angstroms) | | |
|----|---|------------------------|-----------|-----------|
| | | X | Y | Z |
| 1 | C | -0.703798 | -2.464147 | -0.001222 |
| 2 | C | 0.736247 | -2.453367 | 0.000762 |
| 3 | C | 1.422077 | -1.229440 | -0.038221 |
| 4 | C | 0.706733 | 0.005211 | -0.028848 |
| 5 | C | -0.706733 | -0.005213 | 0.028847 |
| 6 | C | -1.408058 | -1.249134 | 0.038029 |
| 7 | C | 1.408057 | 1.249132 | -0.038041 |
| 8 | C | 0.703796 | 2.464143 | 0.001211 |
| 9 | C | -0.736244 | 2.453363 | -0.000748 |
| 10 | C | -1.422075 | 1.229438 | 0.038232 |
| 11 | C | -2.888598 | 1.218467 | 0.018888 |
| 12 | N | -3.525614 | -0.023200 | 0.007529 |
| 13 | C | -2.876441 | -1.262819 | 0.019716 |
| 14 | C | 2.888599 | -1.218467 | -0.018851 |

| | | | | |
|----|---|-----------|-----------|-----------|
| 15 | N | 3.525615 | 0.023201 | -0.007534 |
| 16 | C | 2.876440 | 1.262818 | -0.019756 |
| 17 | N | -1.307921 | -3.698781 | -0.001336 |
| 18 | N | 1.362765 | -3.677581 | -0.000827 |
| 19 | N | 1.307916 | 3.698781 | 0.001285 |
| 20 | N | -1.362760 | 3.677582 | 0.000883 |
| 21 | O | -3.554325 | -2.298335 | 0.010155 |
| 22 | O | 3.594471 | -2.235402 | -0.007346 |
| 23 | O | -3.594465 | 2.235404 | 0.007342 |
| 24 | O | 3.554319 | 2.298337 | -0.010148 |
| 25 | C | -4.993606 | 0.003608 | -0.014608 |
| 26 | C | 4.993606 | -0.003607 | 0.014604 |
| 27 | H | -2.320510 | -3.656002 | -0.088043 |
| 28 | H | -0.834626 | -4.405182 | -0.550155 |
| 29 | H | 0.906275 | -4.390963 | 0.553327 |
| 30 | H | 2.374865 | -3.614607 | 0.084459 |
| 31 | H | 2.320508 | 3.656004 | 0.087978 |
| 32 | H | 0.834633 | 4.405195 | 0.550100 |
| 33 | H | -0.906285 | 4.390976 | -0.553268 |
| 34 | H | -2.374863 | 3.614609 | -0.084388 |
| 35 | H | -5.344232 | -1.023893 | 0.012588 |
| 36 | H | -5.340671 | 0.504922 | -0.920442 |
| 37 | H | -5.363030 | 0.563106 | 0.846638 |
| 38 | H | 5.344233 | 1.023892 | -0.012656 |
| 39 | H | 5.340673 | -0.504863 | 0.920470 |
| 40 | H | 5.363028 | -0.563160 | -0.846606 |

Total energy: -1247.71569169 Hartrees

4. OFET performances of 4NH₂-NDI, DHNDI, and blend system with D/A molar ratio of 1:3

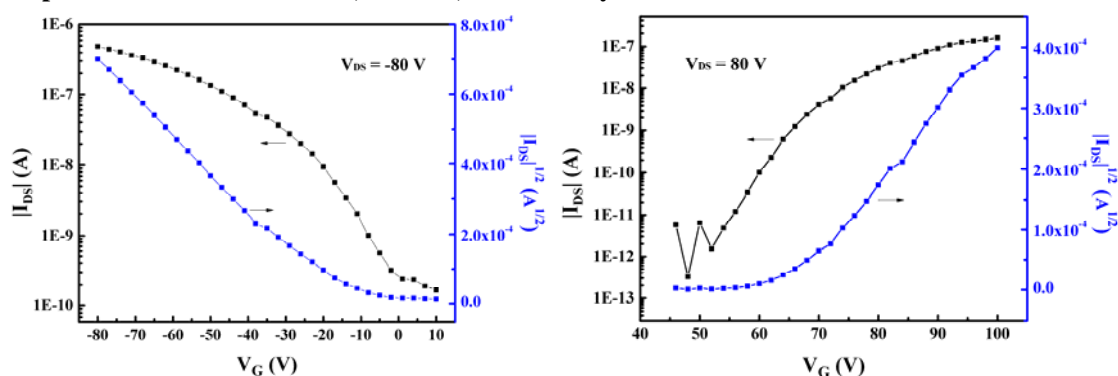


Fig. S3 Transfer characteristics for OFETs of 4NH₂-NDI (left, measured in air) and DHNDI (right, measure in N₂); the channel width (W) and length (L) were 1440 μm and 50 μm , respectively.

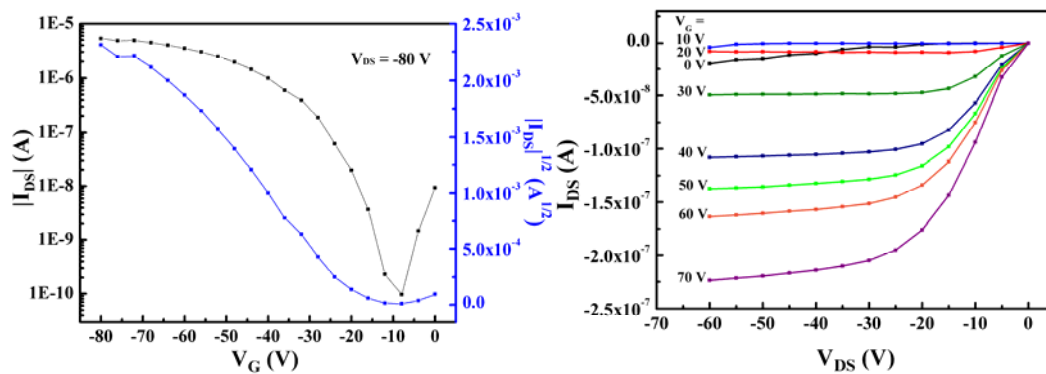


Fig. S4 Transfer (*left*) and output (*right*) characteristics for OFETs of blend system with D/A molar ratio of 1:3 measured in air; the channel width (W) and length (L) were 1440 μm and 50 μm , respectively.

5. AFM images of thin films of 4NH₂-NDI (A) and DHNDI (B) after annealing at different temperatures

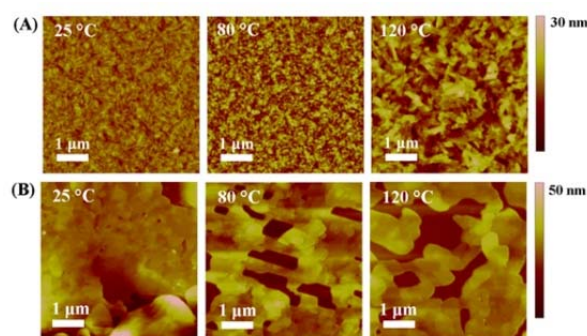


Fig. S5 AFM images of thin films of 4NH₂-NDI (A) and DHNDI (B) after annealing at different temperatures.

6. ¹H NMR and ¹³C NMR spectra of 4NH₂-NDI and compound 1

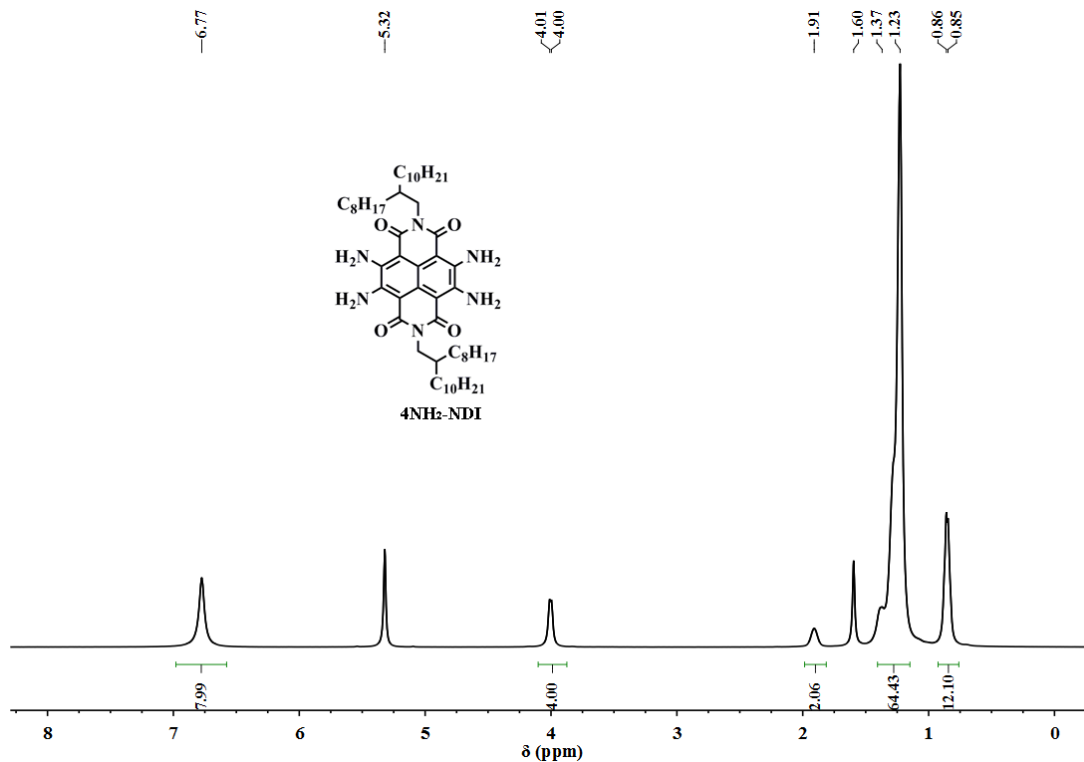


Fig. S6 ¹H NMR spectra of 4NH₂-NDI

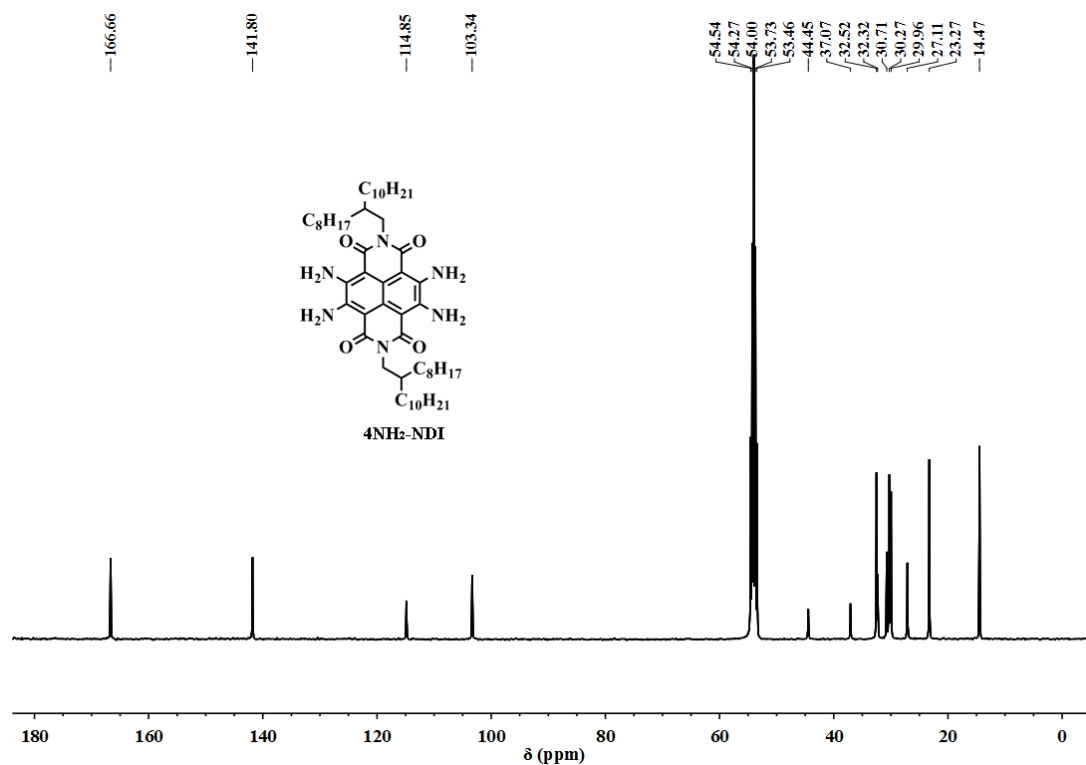


Fig. S7 ¹³C NMR spectra of 4NH₂-NDI

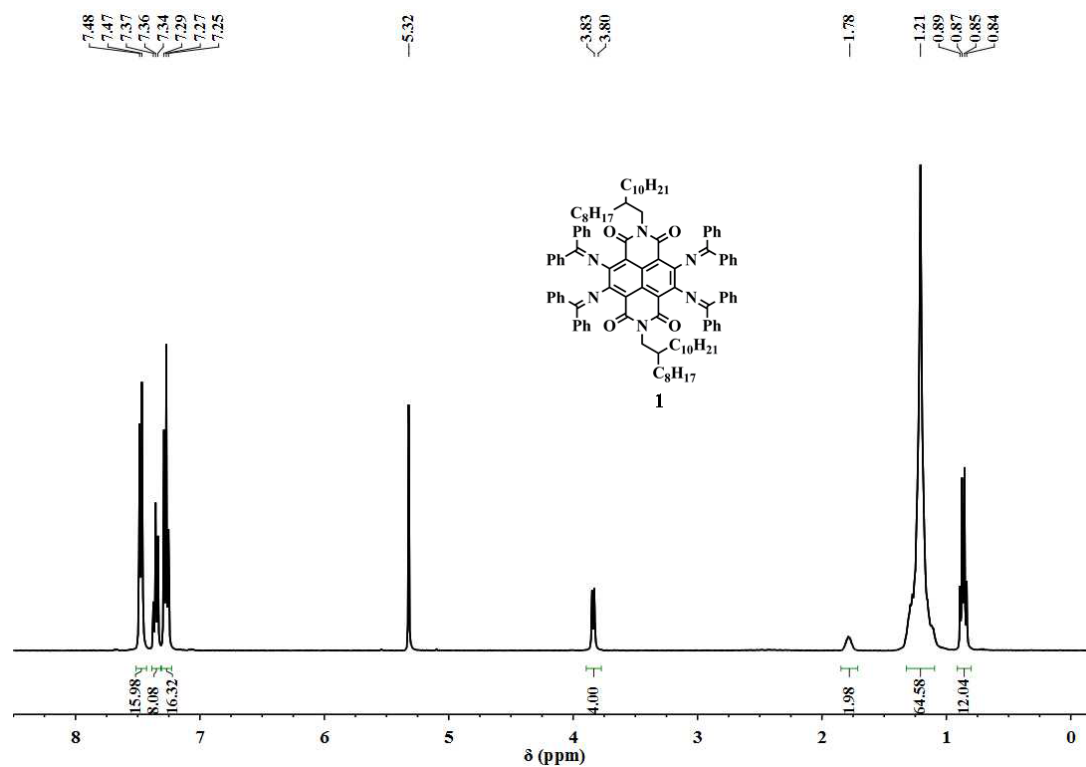


Fig. S8 ¹H NMR spectra of 1

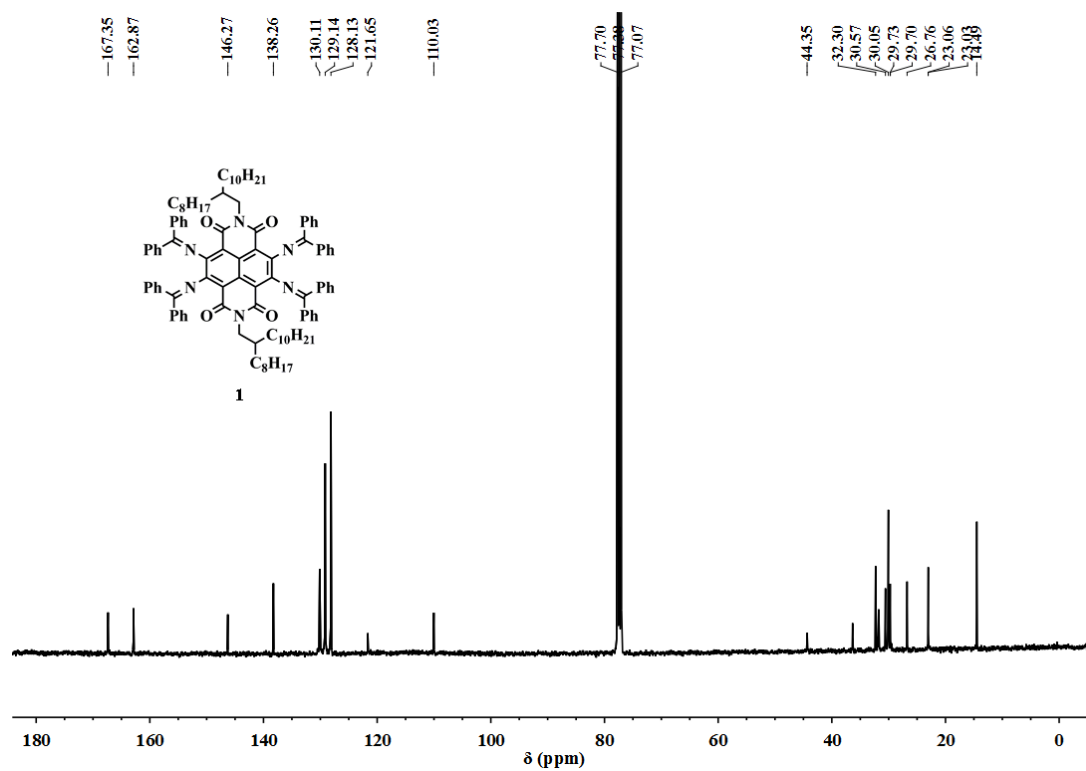


Fig. S9 ¹³C NMR spectra of **1**