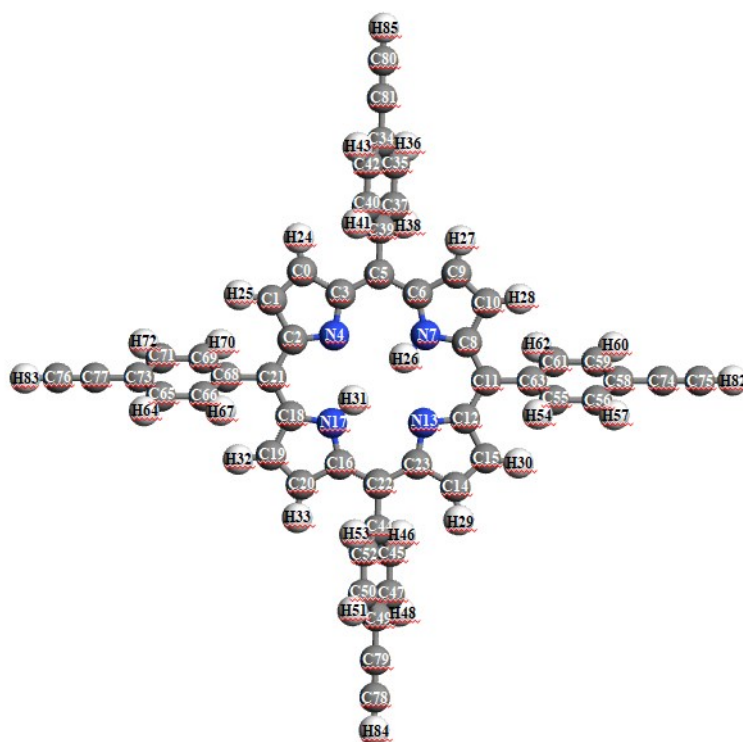


**Title:** Four probe electron transport characteristics of porphyrin phenylacetylene molecule devices

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**The following is supplementary information:**



**Fig S1** the PPA molecule(AB, A=atom; B=atomic number). The numbers in the figure correspond to the numbers in table S1.

**Table S1** the supercell vectors of the systems for optimized PPA.

| Number | Atom | X(Å)    | Y(Å)    | Z(Å)    |
|--------|------|---------|---------|---------|
| 0      | C    | 11.0883 | 23.4445 | 17.9869 |
| 1      | C    | 11.0068 | 22.5084 | 16.9986 |
| 2      | C    | 10.9988 | 21.2119 | 17.6728 |
| 3      | C    | 11.0925 | 22.7037 | 19.2486 |

|    |   |         |         |         |
|----|---|---------|---------|---------|
| 4  | N | 11.0421 | 21.3505 | 19.0361 |
| 5  | C | 11.1277 | 23.3491 | 20.5118 |
| 6  | C | 11.1128 | 22.713  | 21.7744 |
| 7  | N | 11.1747 | 21.3604 | 22.0319 |
| 8  | C | 11.0836 | 21.1284 | 23.3872 |
| 9  | C | 10.9719 | 23.3755 | 23.0459 |
| 10 | C | 10.9492 | 22.4084 | 24.0301 |
| 11 | C | 11.0678 | 19.8625 | 24.0189 |
| 12 | C | 11.0162 | 18.6262 | 23.3203 |
| 13 | N | 10.9646 | 18.4868 | 21.9573 |
| 14 | C | 10.9262 | 16.3912 | 23.0066 |
| 15 | C | 11.0145 | 17.3286 | 23.9941 |
| 16 | C | 10.8833 | 17.1259 | 19.2198 |
| 17 | N | 10.8282 | 18.4789 | 18.9619 |
| 18 | C | 10.9209 | 18.7114 | 17.6071 |
| 19 | C | 11.0473 | 17.4311 | 16.9645 |
| 20 | C | 11.0191 | 16.4636 | 17.948  |
| 21 | C | 10.9447 | 19.9765 | 16.9752 |
| 22 | C | 10.871  | 16.4891 | 20.4825 |
| 23 | C | 10.9131 | 17.1334 | 21.7456 |
| 24 | H | 11.1403 | 24.5312 | 17.8746 |
| 25 | H | 10.9427 | 22.675  | 15.9193 |
| 26 | H | 11.2425 | 20.6095 | 21.331  |
| 27 | H | 10.8654 | 24.4573 | 23.1647 |
| 28 | H | 10.8162 | 22.5446 | 25.1077 |
| 29 | H | 10.8746 | 15.3033 | 23.115  |
| 30 | H | 11.0828 | 17.1639 | 25.0735 |
| 31 | H | 10.7641 | 19.2315 | 19.661  |
| 32 | H | 11.1816 | 17.2899 | 15.8882 |
| 33 | H | 11.1205 | 15.3818 | 17.826  |
| 34 | C | 11.1046 | 27.6836 | 20.5864 |
| 35 | C | 12.2446 | 26.9657 | 21.0169 |
| 36 | H | 13.1271 | 27.5183 | 21.3706 |
| 37 | C | 12.2518 | 25.5671 | 20.989  |
| 38 | H | 13.1488 | 25.0157 | 21.3102 |
| 39 | C | 11.1279 | 24.8452 | 20.5351 |
| 40 | C | 9.99121 | 25.5652 | 20.1126 |
| 41 | H | 9.10331 | 25.0091 | 19.7763 |
| 42 | C | 9.97475 | 26.9627 | 20.1347 |
| 43 | H | 9.07834 | 27.5106 | 19.8116 |
| 44 | C | 10.8669 | 14.9927 | 20.4595 |
| 45 | C | 12.0027 | 14.2664 | 20.8745 |
| 46 | H | 12.8947 | 14.8178 | 21.2074 |
| 47 | C | 12.0116 | 12.8686 | 20.854  |

|    |   |         |         |         |
|----|---|---------|---------|---------|
| 48 | H | 12.9064 | 12.3163 | 21.1752 |
| 49 | C | 10.8756 | 12.153  | 20.4086 |
| 50 | C | 9.73605 | 12.8773 | 19.9873 |
| 51 | H | 8.84607 | 12.3308 | 19.6431 |
| 52 | C | 9.73687 | 14.2758 | 20.014  |
| 53 | H | 8.83944 | 14.8304 | 19.7006 |
| 54 | H | 9.20602 | 18.7666 | 25.7011 |
| 55 | C | 10.04   | 19.2356 | 26.2457 |
| 56 | C | 10.0525 | 19.2281 | 27.6437 |
| 57 | H | 9.24367 | 18.7429 | 28.2085 |
| 58 | C | 11.0982 | 19.8593 | 28.3563 |
| 59 | C | 12.1347 | 20.4875 | 27.6284 |
| 60 | H | 12.9556 | 20.9707 | 28.1773 |
| 61 | C | 12.1204 | 20.4819 | 26.2302 |
| 62 | H | 12.9418 | 20.9602 | 25.6745 |
| 63 | C | 11.0766 | 19.8557 | 25.5106 |
| 64 | H | 9.06499 | 18.8727 | 12.8129 |
| 65 | C | 9.88541 | 19.3545 | 13.3643 |
| 66 | C | 9.89461 | 19.3612 | 14.7625 |
| 67 | H | 9.06864 | 18.8885 | 15.3161 |
| 68 | C | 10.9397 | 19.9821 | 15.4847 |
| 69 | C | 11.9825 | 20.596  | 14.7544 |
| 70 | H | 12.8165 | 21.0603 | 15.303  |
| 71 | C | 11.9759 | 20.6023 | 13.3567 |
| 72 | H | 12.792  | 21.08   | 12.7963 |
| 73 | C | 10.9285 | 19.9771 | 12.641  |
| 74 | C | 11.0954 | 19.8649 | 29.7885 |
| 75 | C | 11.0739 | 19.8652 | 31.0115 |
| 76 | C | 10.9684 | 19.9587 | 9.98687 |
| 77 | C | 10.94   | 19.9647 | 11.2097 |
| 78 | C | 10.8896 | 9.49835 | 20.3657 |
| 79 | C | 10.882  | 10.7212 | 20.3854 |
| 80 | C | 11.0746 | 30.3372 | 20.6384 |
| 81 | C | 11.0917 | 29.1148 | 20.6072 |
| 82 | H | 11.0478 | 19.8769 | 32.0903 |
| 83 | H | 10.9965 | 19.9469 | 8.90846 |
| 84 | H | 10.9009 | 8.41964 | 20.3443 |
| 85 | H | 11.0579 | 31.4156 | 20.6611 |

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