Electronic Supplementary Information (ESI) for

“How to tune efficiently the biradicaloid nature of acenes by chemical doping with boron and nitrogen”

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(Dated: June 23, 2017)

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VII. Cartesian coordinates
## I. MOLECULAR GEOMETRY OF PRISTINE ACENES

TABLE S1: Geometrical parameters (bond lengths, Å) of the pristine tetracene (C_{18}H_{12}) and octacene (C_{34}H_{20}) molecules calculated at the restricted MP2/def2-TZVP level using the resolution of identity approximation. Theoretical DFT-B3LYP (with 6-311++G(d,p) basis set for tetracene and 6-31G* for octacene) results and experimental data for tetracene obtained from x-ray crystallography measurements are included for comparison.

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<th>octacene</th>
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\(^{d}\) Yang, Y.; Davidson, E. R.; Yang, W. PNAS 2016, 113, E5098-E5107.
II. EFFECTS OF DOPING ON MOLECULAR STRUCTURES

TABLE S2: Local effect of the double boron substitution on the molecular structure of tetracene and octacene resulting from MP2/def2-TZVP geometry optimization. The bond length difference ($\Delta R = R^{\text{doped}}_{i} - R^{\text{pristine}}_{i}$) with respect to the optimized pristine oligomers are given in parentheses. $R_1$ and $R_3$ are ladder B-C bonds located on the long molecular axis, while $R_2$ correspond to the rung bonds for the $\alpha$ and $\gamma$ configurations and the B-H bonds in the case of $\beta$. All values are given in Å.

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<td>1.196 (0.112)</td>
<td>1.535 (0.164)</td>
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<tr>
<td>4,13</td>
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<td>1.540 (0.116)</td>
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<td>1.510 (0.106)</td>
<td>1.636 (0.185)</td>
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**B2-octacene** ($C_{32}H_{20}B_2$)

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**N2-octacene** ($C_{32}H_{20}N_2$)

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**N2-tetracene** ($C_{16}H_{12}N_2$)

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<td>1.370 (-0.031)</td>
<td>1.403 (-0.061)</td>
<td>1.370 (-0.031)</td>
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TABLE S3: Local effect of the double nitrogen substitution on the molecular structure of tetracene and octacene as given by MP2/def2-TZVP geometry optimization. The bond length difference ($\Delta R = R^{\text{doped}}_{i} - R^{\text{pristine}}_{i}$) with respect to the optimized pristine oligomers are given in parentheses. $R_1$ and $R_3$ are ladder C-N bonds located on the long molecular axis, while $R_2$ correspond to the rung bonds for the $\alpha$ and $\gamma$ configurations and the N-H bonds in the case of $\beta$. All values are given in Å.
FIG. S1: The bond alternation patterns ($R_i - 1.4$), in Å, is shown for a boron and b nitrogen doped octacene at two different $\alpha$ (5,22 and 9,26) and $\beta$ (3,20 and 10,27) configurations. Comparison between the geometries of pristine molecule (right panels) and doped systems reveals that a the B-C bond lengths are stretched, while the b N-C bond lengths are slightly shortened; in all cases the geometry distortions propagate away from the doping sites. The coordinates of the bonds, $x$, are given by the average between the coordinates of two successive atoms involved in each bond. Horizontal dashed lines representing the highest (1.464 Å) and lowest (1.370 Å) bond distances of the pristine system are drawn to facilitate comparisons.
III. NATURAL ORBITALS OCCUPATION NUMBERS

FIG. S2: Evolution of the natural orbitals occupation numbers along the series of dual-doped oligoacenes obtained from MR-AQCC calculations.
FIG. S3: **a**, Evolution of the total number of effectively unpaired electrons ($N_U$) and its atomic compositions calculated from MR-AQCC density for the series of dual-doped tetracenes, which demonstrates the wide range of polyradical character achievable. The horizontal dashed line corresponds to reference value of $N_U = 0.5e$ obtained for the pristine tetracene. **b**, The unpaired electron densities plotted at a 0.002 u.a. isosurface level indicate the spatial regions of higher polyradical character.
V. MULLIKEN NET CHARGES OF $\sigma$-SYSTEM

FIG. S4: a, Mulliken net $\sigma$-charges calculated at the HF theory level for the series of dual-doped octacene structures. b, Color-scale mapping of Mulliken net $\sigma$ charges.
VI. EFFECTS OF DOPING ON NATURAL ORBITALS LOCALIZATION

FIG. S5: Evolution of the natural orbitals localization along the series of dual-doped octacene obtained from MR-AQCC calculations.
VII. CARTESIAN COORDINATES

The list of cartesian geometries for all pristine and doped structures optimized at RI-MP2/def2-TZVP level is given below. The electronic $\pi$ charge ($q_\pi$) and the effective number of unpaired electrons ($N_U$), as obtained by the Mulliken analysis of the AQCC electronic density, is also included in the list below.

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### 3,12 B2-tetracene (C\textsubscript{16}B\textsubscript{2}H\textsubscript{12})

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### 5,14 B2-tetracene (C$_{16}$B$_2$H$_{12}$)

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7,16 B2-tetracene (C_{16}B_{2}H_{12})

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5,14 N2-tetracene (C$_{16}$N$_2$H$_{12}$)

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7,24 B2-octacene (C$_{18}$B$_{2}$H$_{20}$)

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8.25 N2-octacene (C₃₄H₂₁N₂)

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