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# SUPPLEMENTARY INFORMATION

## Anti-Ohmic single molecule electron transport: Is it feasible?

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**Reviewing the chemical view of a TI in the model of polyacetylene.**

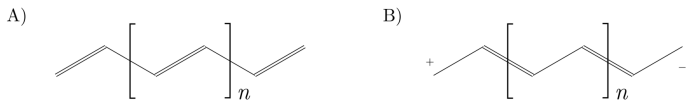



Figure S1: Resonant forms of polyacetylene: A) *trivial*, B) *topological*

In Fig. S1, two different resonance forms of polyacetylene are shown. In form (A) (the *trivial* case), the bonding of the carbon skeleton is simply represented by alternating double and single bonds. In this figure, t and t' represents, as mentioned in the methodology section, the double and single bond intensities, respectively, with t>t'. It was shown using the Hückel formalism that, in this resonance form, the frontier orbitals become strongly delocalized along the carbon frame and display a relevant orbital energy gap. On the contrary, form (B) (the *topological* case) is a structure with the charge polarized at the terminal carbons and the single and double bond character inverted, leading to a situation where t<t'. As a result, in form (B) the frontier orbitals become strongly localized at the edges of the chain and display a zero-energy gap. However, the valence and conduction bands formed by the rest of occupied and virtual states are still significantly separated in energy as in form (A), with the HOMO and LUMO states located in the middle of this band gap. Therefore, in form (B) the system behaves as a conductor only at the edges of the chain but remains insulator in the rest. This is the main characteristic of a TI when it is confined to one dimension.

**Calculation of the delocalization indeces in a Multireference scenario.**

Defining the following matrices,

$$(PS)^{HL}_{\mu\nu} = \sum_{\lambda} C^H_\mu C^L_\lambda S_{\lambda\nu} \tag{1}$$

$$(PS)^{H}_{\mu\nu} = \sum_{\lambda} C^H_\mu C^H_\lambda S_{\lambda\nu} \tag{2}$$

where $C^H_\mu$, $C^H_\lambda$ and $C^L_\lambda$ represent coefficients of the basis functions $\mu$ and $\lambda$ in the HOMO and LUMO orbitals and $S_{\lambda\nu}$ the corresponding overlap integral between these basis, and their counterparts, $\mathbf{PS}^{LH}$ and $\mathbf{PS}^{L}$, expressions of the Mulliken type electron delocalization index for each state are straightforwardly obtained,

$$\delta_1^S(A,B) = c^2 \sum_{\mu\in A}\sum_{\nu\in B}(PS)^H_{\mu\nu}(PS)^H_{\nu\mu} + (1-c^2)\sum_{\mu\in A}\sum_{\nu\in B}(PS)^L_{\mu\nu}(PS)^L_{\nu\mu} + 2c(1-c^2)^{1/2}\sum_{\mu\in A}\sum_{\nu\in B}\left[(PS)^H_{\mu\nu}(PS)^{LH}_{\nu\mu}(PS)^L_{\mu\nu}(PS)^{HL}_{\nu\mu}\right] \tag{3}$$

$$\delta_2^S(A,B) = (1-c^2)\sum_{\mu\in A}\sum_{\nu\in B}(PS)^H_{\mu\nu}(PS)^H_{\nu\mu} + c^2\sum_{\mu\in A}\sum_{\nu\in B}(PS)^L_{\mu\nu}(PS)^L_{\nu\mu} - 2c(1-c^2)^{1/2}\sum_{\mu\in A}\sum_{\nu\in B}\left[(PS)^H_{\mu\nu}(PS)^{LH}_{\nu\mu}(PS)^L_{\mu\nu}(PS)^{HL}_{\nu\mu}\right] \tag{4}$$

$$\delta_3^S(A,B) = (1/2)\left[\sum_{\mu\in A}\sum_{\nu\in B}(PS)^H_{\mu\nu}(PS)^H_{\nu\mu} + \sum_{\mu\in A}\sum_{\nu\in B}(PS)^L_{\mu\nu}(PS)^L_{\nu\mu}\right] + \left[\sum_{\mu\in A}\sum_{\nu\in B}(PS)^H_{\mu\nu}(PS)^{LH}_{\nu\mu}(PS)^L_{\mu\nu}(PS)^{HL}_{\nu\mu}\right] \tag{5}$$

$$\delta^T(A,B) = (1/2)\left[\sum_{\mu\in A}\sum_{\nu\in B}(PS)^H_{\mu\nu}(PS)^H_{\nu\mu} + \sum_{\mu\in A}\sum_{\nu\in B}(PS)^L_{\mu\nu}(PS)^L_{\nu\mu}\right] - \left[\sum_{\mu\in A}\sum_{\nu\in B}(PS)^H_{\mu\nu}(PS)^{LH}_{\nu\mu}(PS)^L_{\mu\nu}(PS)^{HL}_{\nu\mu}\right] \tag{6}$$

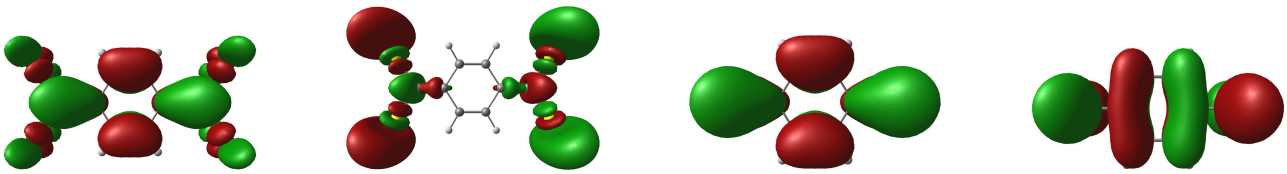
In order to calculate the **PS** matrices a molecular orbital basis must be introduced. A first choice is indeed the HF or KS orbitals from the one-determinant closed-shell calculation, both giving, in this case, the same result.

**Effect of the hydrogenation of pX2 in the properties obtained with gold**

As it has been observed in the Fig. 6 of the Main Article, the significant long-range electron exchange between terminal rings displayed by chains including gold is reinforced in the hydrogenated chains. This is not the only property that remains unchanged, as it can be observed in Table S1, the Energy Gap tendency of the **pX2** structures is kept so as the closeness of its values. In addition the orbital dsitribution is also equal for the hydrogenated and golden chains as can be observed in Fig. S2-S6, the representation of this orbitals were performed with the Chemcraft software with an isovalue=3E-2 (default) for all the plots.

Table S1: HOMO-LUMO Gaps of the phenyl **pX2** structures with H and Au atoms from $n$=1-12

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ΔE\eV (**pX2** with H) | 3.73 | 2.21 | 1.37 | 0.74 | 0.34 | 0.18 | 0.13 | 0.09 | 0.08 | 0.07 | 0.07 | 0.06 |
| ΔE\eV (**pX2** with Au) | 3.11 | 1.91 | 1.16 | 0.60 | 0.28 | 0.16 | 0.12 | 0.09 | 0.08 | 0.07 | 0.06 | 0.06 |



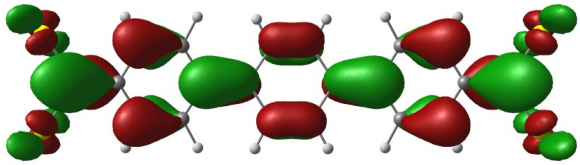
(a) HOMO orbital of the Au substituted molecule

(b) LUMO orbital of the Au substituted molecule

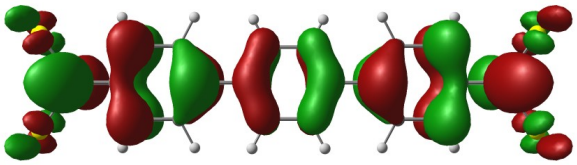
(c) HOMO orbital of the H substituted molecule

(d) LUMO orbital of the H substituted molecule

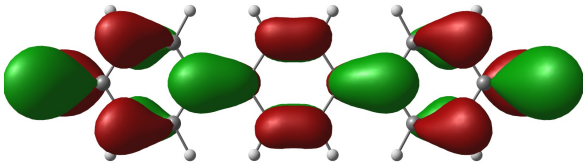
Figure S2: **pX2** with $n$=1 phenyl rings with Au or H atoms



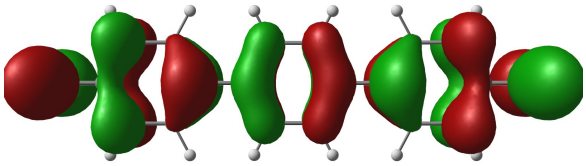
(a) HOMO orbital of the Au substituted Molecule



(b) LUMO orbital of the Au substituted Molecule

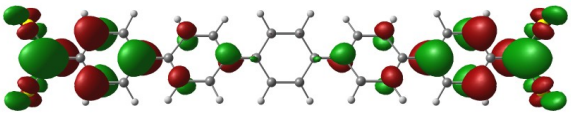


(c) HOMO orbital of the H substituted Molecule

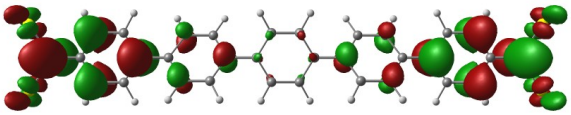


(d) LUMO orbital of the H substituted Molecule

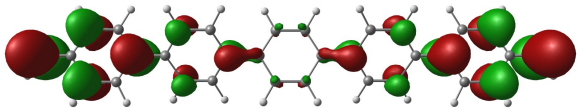
Figure S3: **pX2** with $n$=3 phenyl rings with Au or H atoms



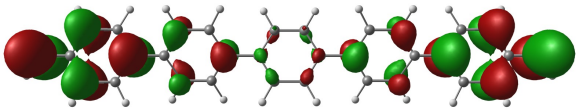
(a) HOMO orbital of the Au substituted Molecule



(b) LUMO orbital of the Au substituted Molecule

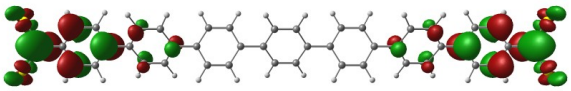


(c) HOMO orbital of the H substituted Molecule

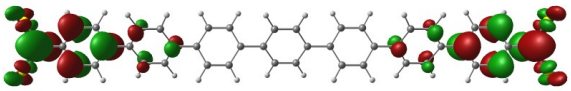


(d) LUMO orbital of the H substituted Molecule

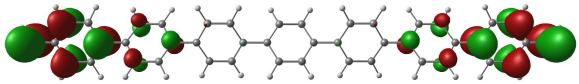
Figure S4: **pX2** with $n$=5 phenyl rings with Au or H atoms



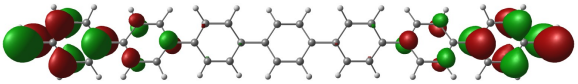
(a) HOMO orbital of the Au substituted Molecule



(b) LUMO orbital of the Au substituted Molecule

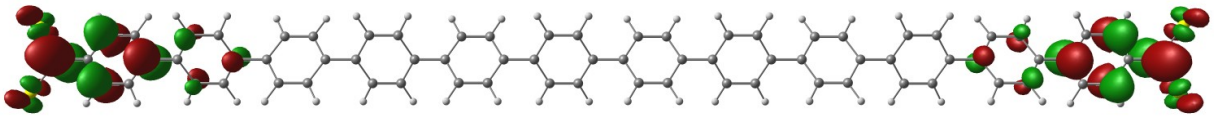


(c) HOMO orbital of the H substituted Molecule

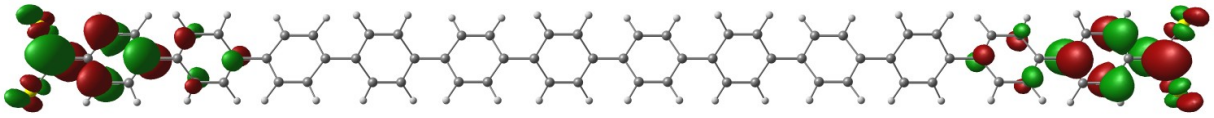


(d) LUMO orbital of the H substituted Molecule

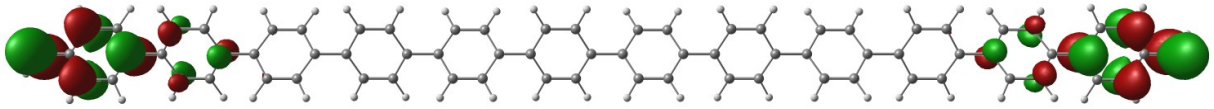
Figure S5: **pX2** with $n$=7 phenyl rings with Au or H atoms



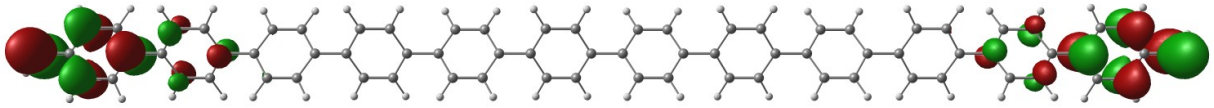
(a) HOMO orbital of the Au substituted Molecule



(b) LUMO orbital of the Au substituted Molecule



(c) HOMO orbital of the H substituted Molecule



(d) LUMO orbital of the H substituted Molecule

Figure S6: **pX2** with $n$=12 phenyl rings with Au or H atoms