Electronic Supplementary Material (ESI) for RSC Advances

Supplementary Information

Design of Hybrid Conjugates Based on Chemical Similarity

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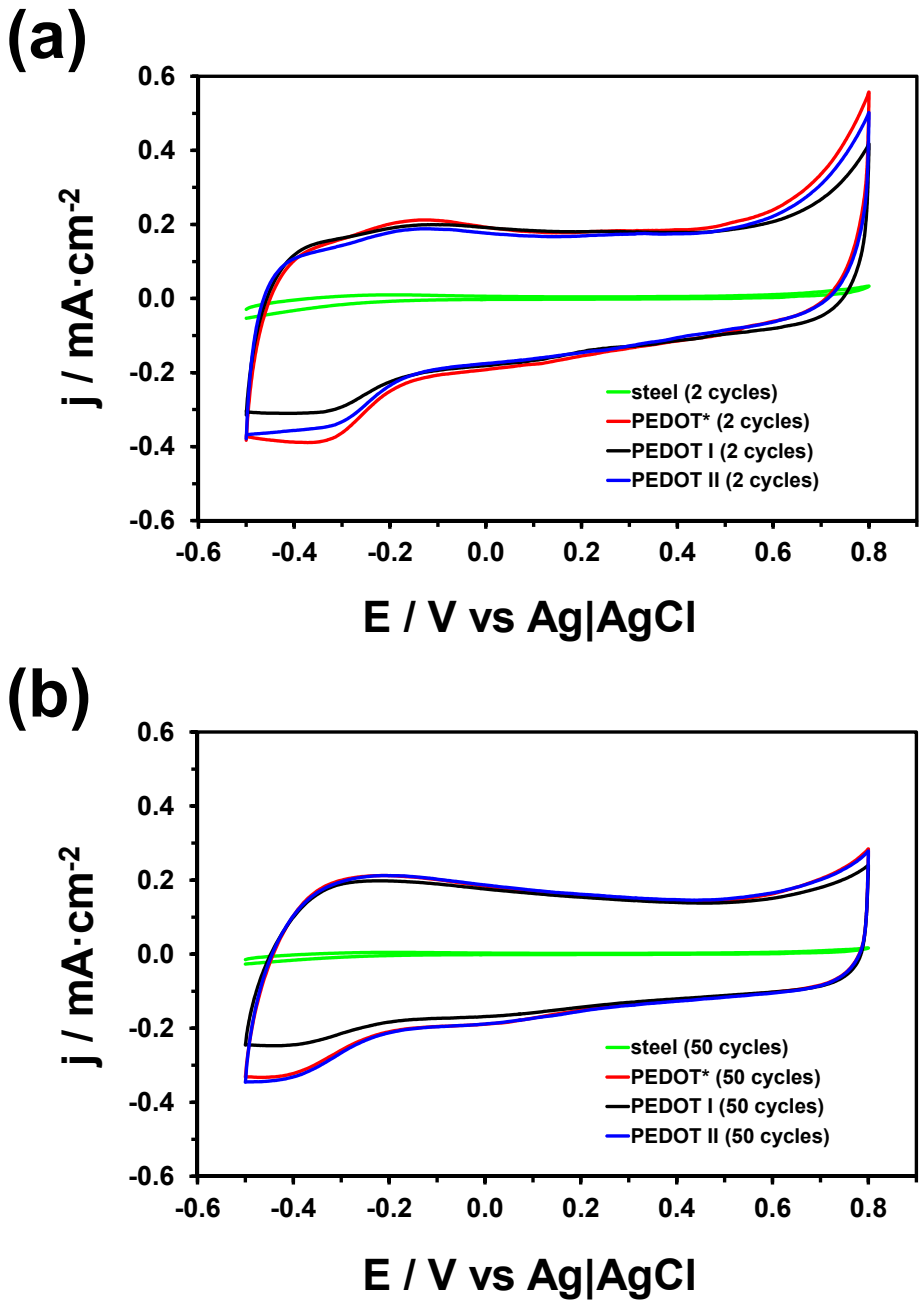

Figure S1. (a) Control voltammograms for PEDOT*, PEDOT-I and PEDOT-II after (a) 2 and (b) 50 consecutive oxidation-reduction cycles. Voltammograms were recorded in a 0.1 M PBS solution at 25 mV/s and 25ºC. Initial and final potentials: –0.50 V; reversal potential: +0.80 V. The reduction peak at -0.4 V has been attributed to the reduction of oxygen.

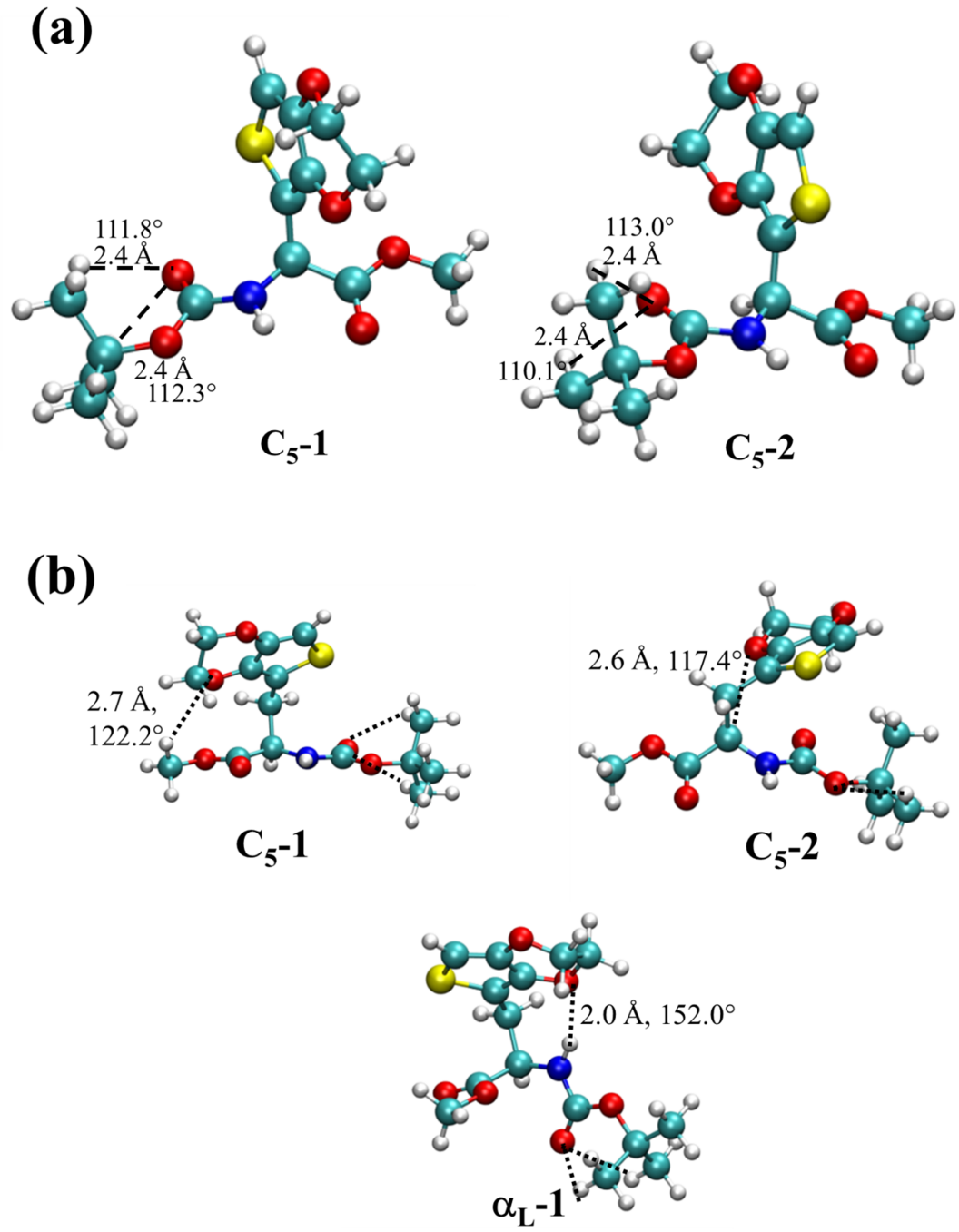

Figure S2. Minimum energy conformations of representative minima of (a) **II** and (b) **I** calculated at the ωB97X-D/6-311++G(d,p) level. The intramolecular interactions are indicated by dashed lines. Geometric parameters associated to these interactions (*i.e.* H···O distance and ∠N/C–H···O angle in hydrogen are indicated.

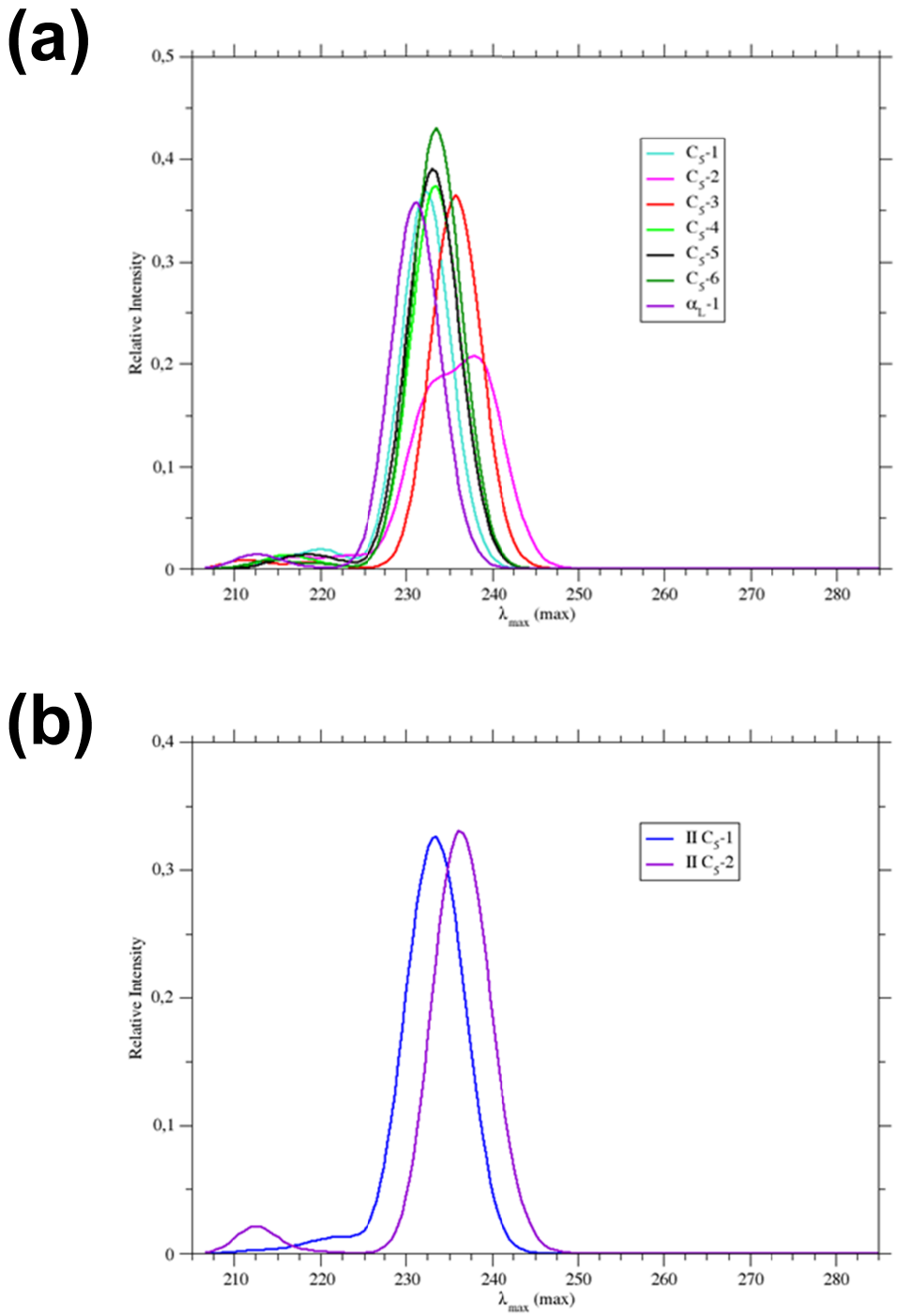

Figure S3. Electronic spectra calculated for the more stable conformations (*i.e.* ΔG < 1.5 kcal/mol; see Tables 5 and 6) of **I** (a) and **II** (b).

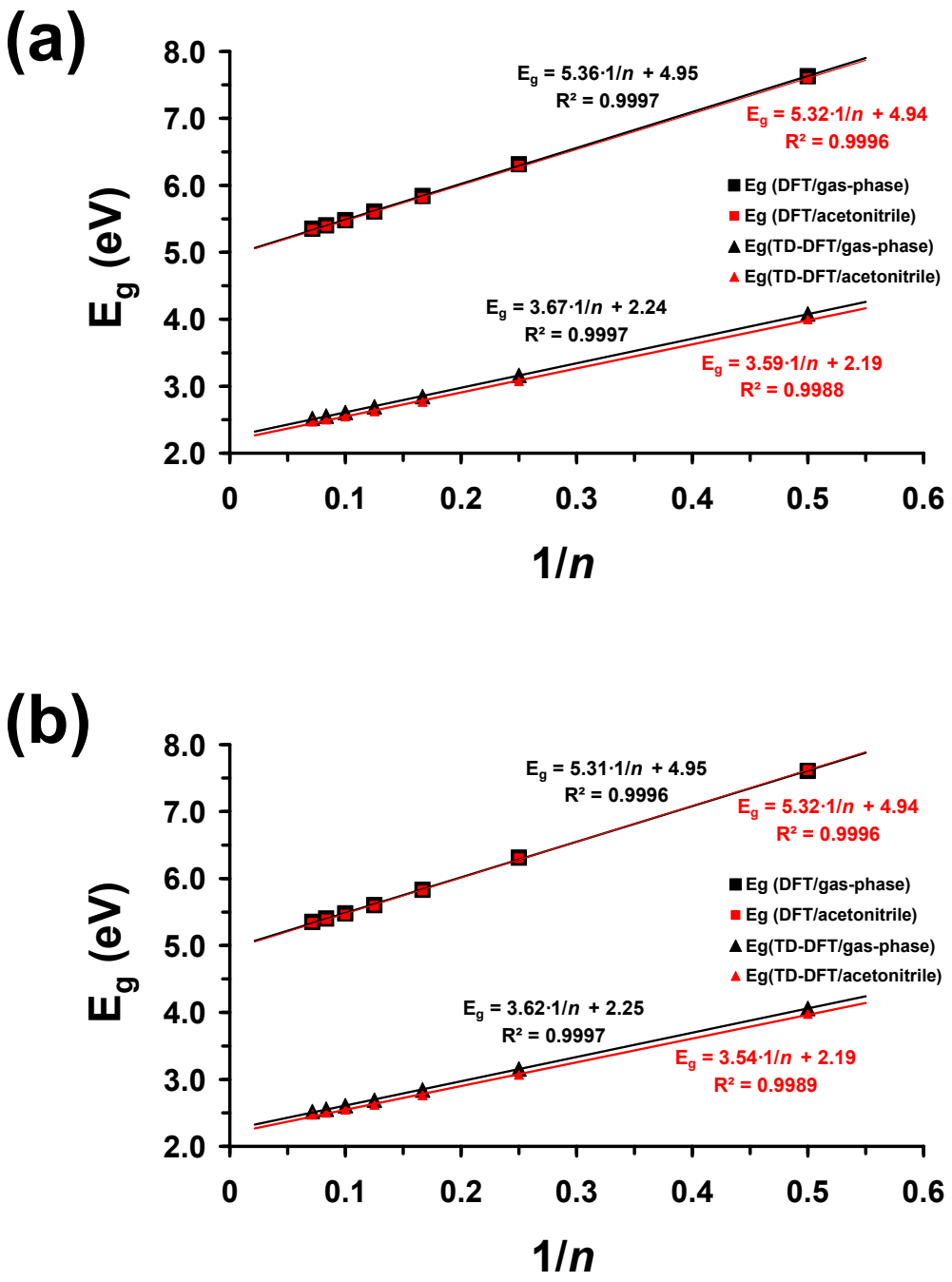

Figure S4. Variation of the E_g derived from both DFT and TD-DFT calculations in the gas-phase (black) and acetonitrile solution (red) against 1/*n*, where *n* is the number of EDOT units, in (a) $(EDOT)_n$-I and (b) $(EDOT)_n$-II. The solid lines correspond to the linear regressions used to extrapolate this electronic property towards conjugates with infinite PEDOT chains.

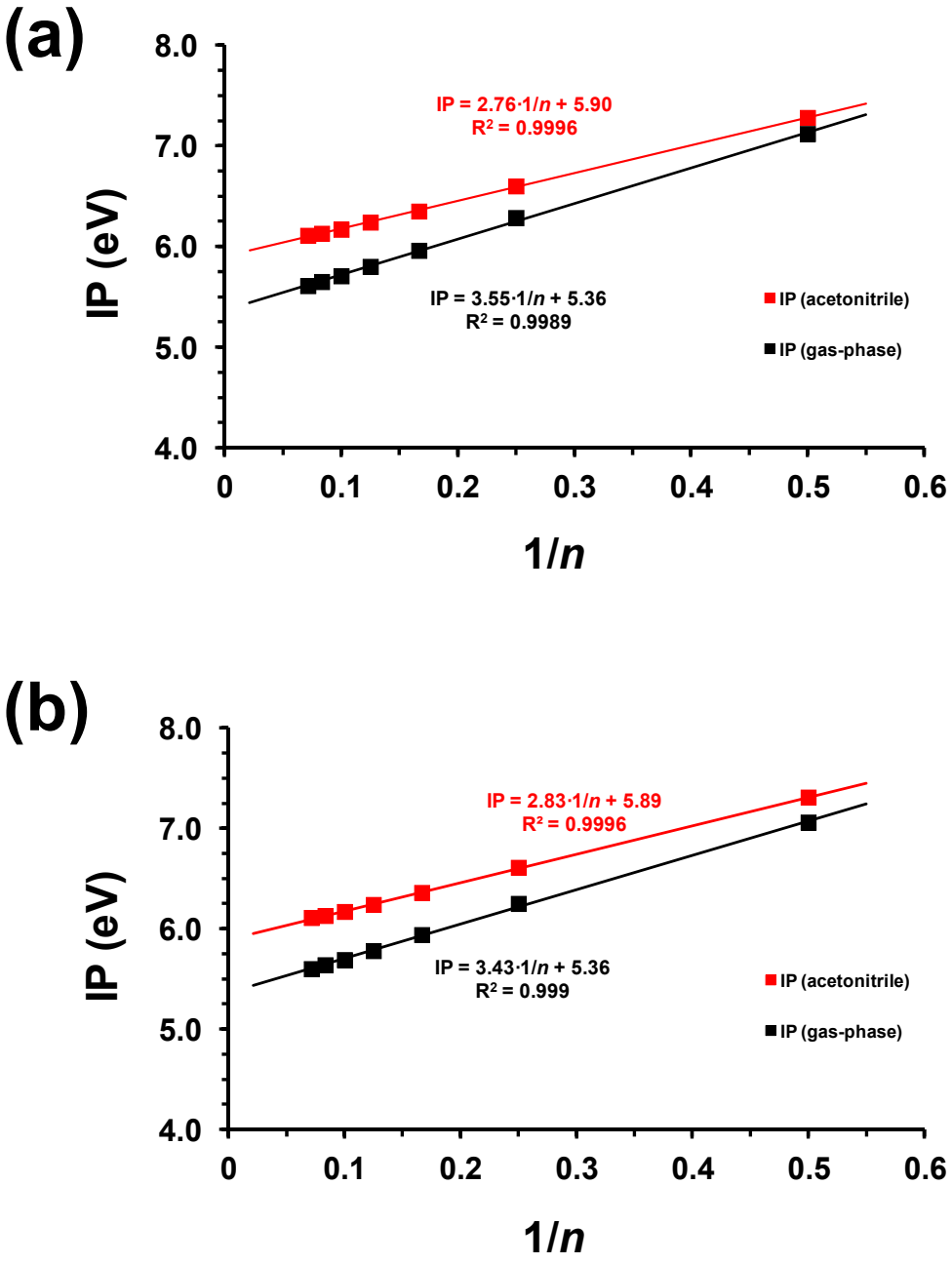

Figure S5. Variation of the IP derived from DFT calculations in the gas-phase (black) and acetonitrile solution (red) against 1/*n*, where *n* is the number of EDOT units, in (a) $(EDOT)_n$-I and (b) $(EDOT)_n$-II. The solid lines correspond to the linear regressions used to extrapolate this electronic property towards conjugates with infinite PEDOT chains.