Supplementary Information Mechanistic studies of hydrogen evolution reaction on donor-acceptor conjugated polymer photocatalysts.

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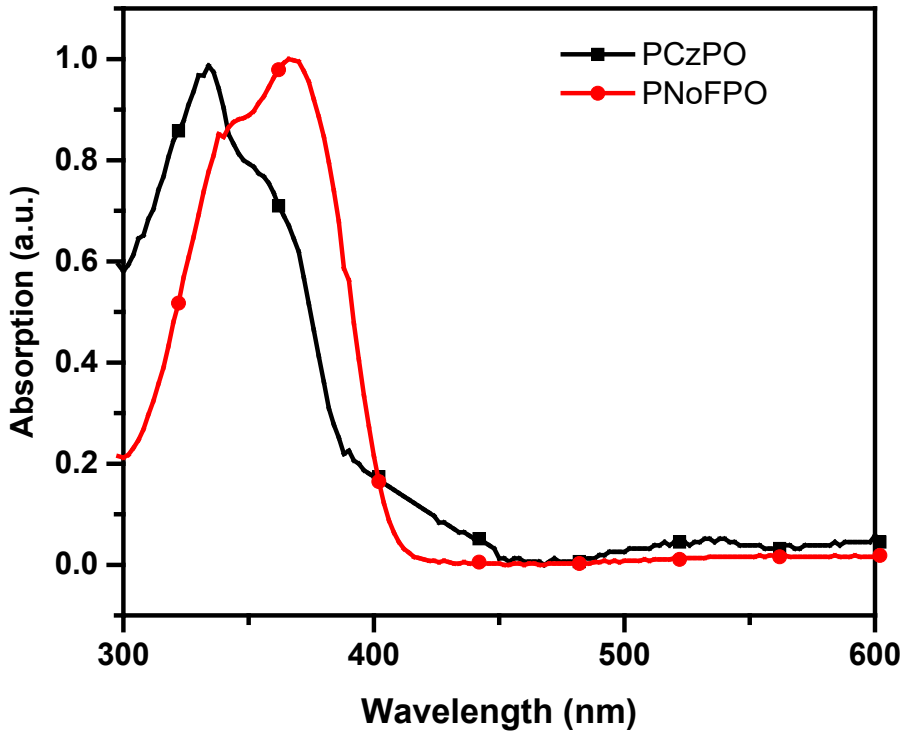

Figure S1. UV-vis absorption spectra of PCzPO and PNoFPO D-A polymers, measured in Dichloromethane.

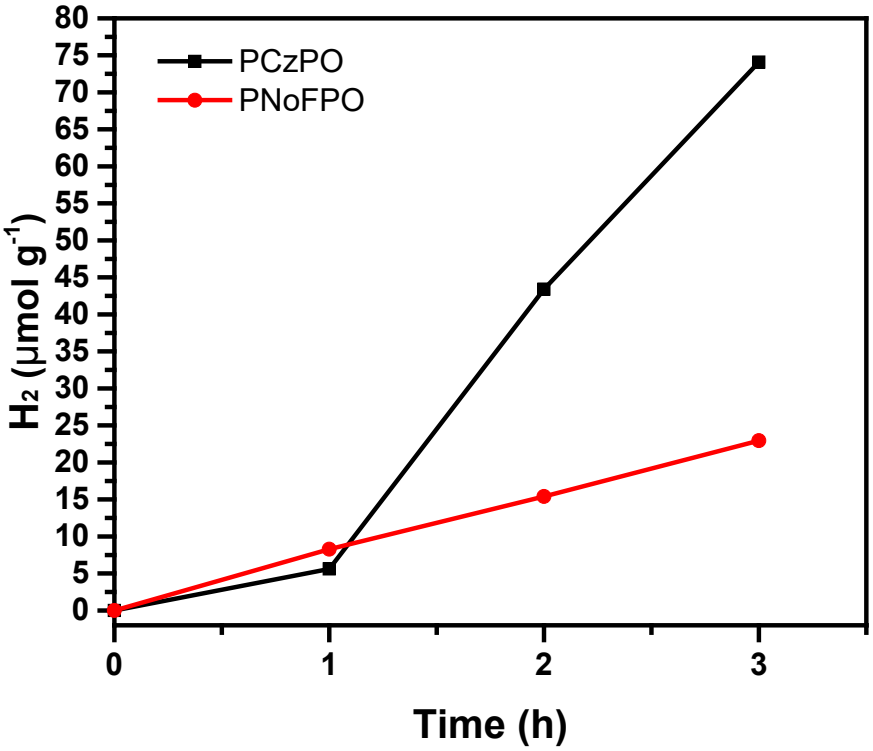

Figure S2. Hydrogen evolution profile of PCzPO and PNoFPO using visible light for polymers (5 mg catalyst in 10 mL mixture (water : MeOH : triethylamine = 1:1:1), 1000 W/m^2, 380 nm – 780 nm, 90 µL H_2PtCl_6 (1M) was added).

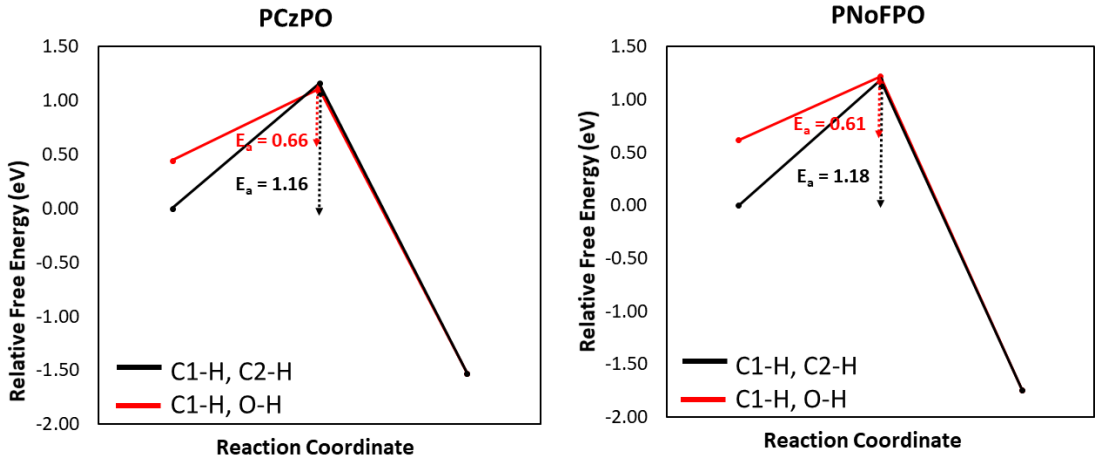

Figure S3. Energy diagram of intramolecular H_2 formation using the PCzPO (left) and PNoFPO (right) D-A moiety models, computed by DFT.

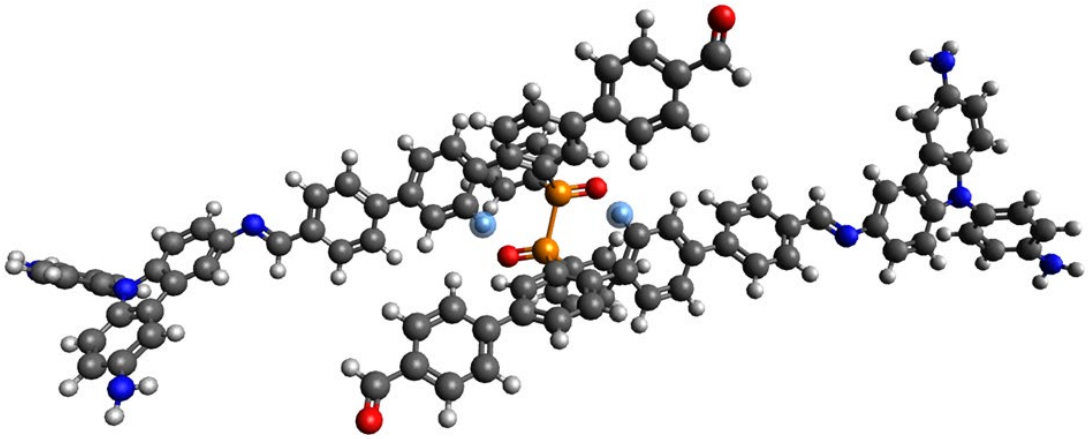

Figure 4. Formation of a phosphorous-phosphorous bond (P atoms are shown as orange spheres and the bond is shown as an orange line) preventing the interaction of bound H atoms (highlighted in light blue) for a complete hydrogen evolution, computed by DFT.