Supporting Information

Single Crystalline Submicrotube from Small Organic Molecule

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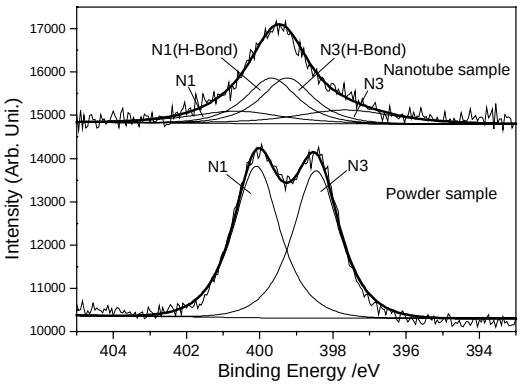
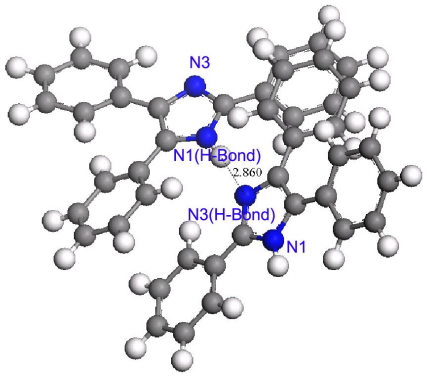
A. N1s XPS of TPI powder sample (the bottom curves) and the tube sample that was dropped onto silicon wafer (the top curves). There are two typical peaks with area ratio about 1:1 in the powder sample, which can well be assigned to N1 (400.09eV) and N3 (398.45eV) respectively. Both the N1 peak and the N3 one split into two peaks in the tube sample. The theoretical calculation results gives that the ionization potentials (IP) of the two H-Bonded nitrogen atoms, N-H…N, are much closer than in the case of monomer, while the IPs of non-hydrogen bonded nitrogen atoms shift away from the position of monomer. So the four peaks in the tube sample (a) can be well contributed to the four corresponding N atoms (b). This is another evidence for the formation of molecular chains through H-Bonds in the submicrotubes.

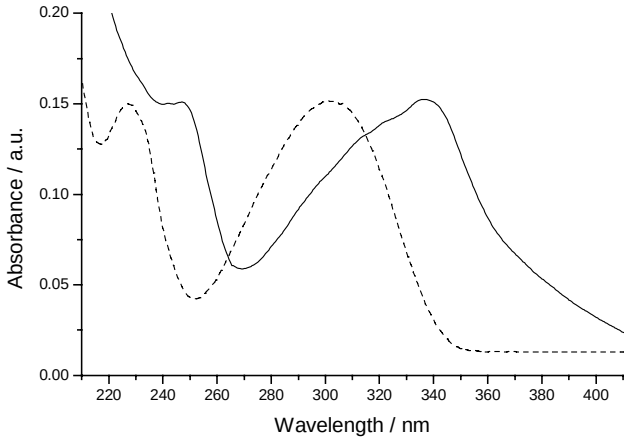


a



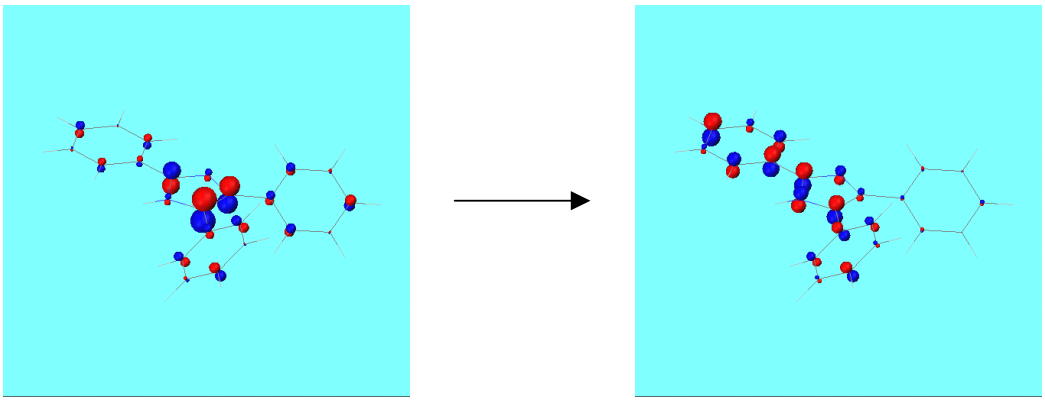
b

B. UV-visible absorption spectra of TPI monomers (dashed line) and TPI tubes with a diameter of 250 nm (solid line). The results were discussed in the text.



C. The assignation of the absorption band of TPI monomer at 302nm (4.10eV) to the transition from S_0 to S_1 (from HOMO to LUMO). The state, configuration and the oscillator strength in the absorption of TPI calculated with ZINDO are listed in the table. The calculated results of the transition energy wavelength are accordant well with the experimental results (4.10eV and 302nm respectively).

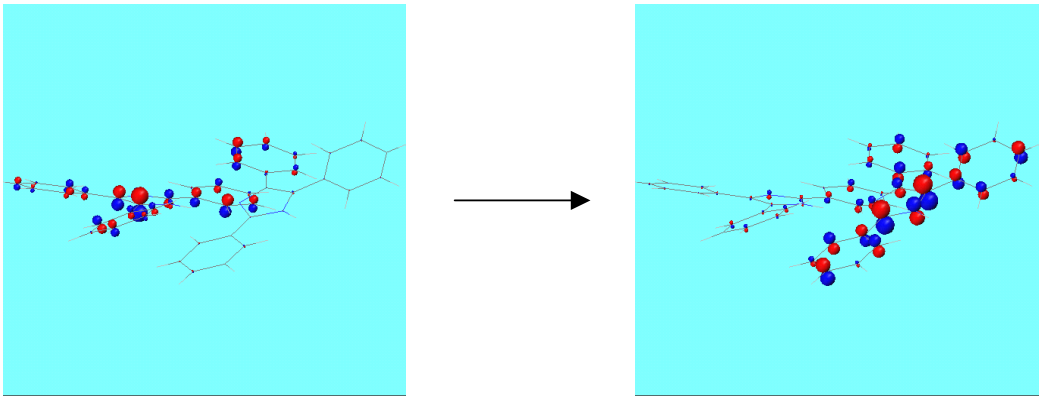
State	Configuration and weight	Transition energy (eV)	Wavelength (nm)	Oscillator strength
$S_0 \rightarrow S_1$	HOMO $\rightarrow$ LUMO (88.78%)	3.920	316.3	0.91



HOMO (π orbital) LUMO (π* orbital)

D. The contribution of the newly arisen band in the absorption spectra of TPI tubes to the transition of $S_0 \rightarrow S_1$. The transition can induce the intermolecular charge transfer (Inter-CT) between the TPI molecules in the neighboring H-Bonded molecular chains, which can be observed from the wave functions of the correlative molecular orbitals.

State	Configurations and weights	Transition energy (eV)	Wavelength (nm)	Oscillator strength
$S_0 \rightarrow S_1$	HOMO $\rightarrow$ LUMO (88.69%)	3.621	342.4	0.90



HOMO LUMO