

Supporting Information

A First Principles Study of the Nuclear Dynamics of Doped Conjugated Polymers

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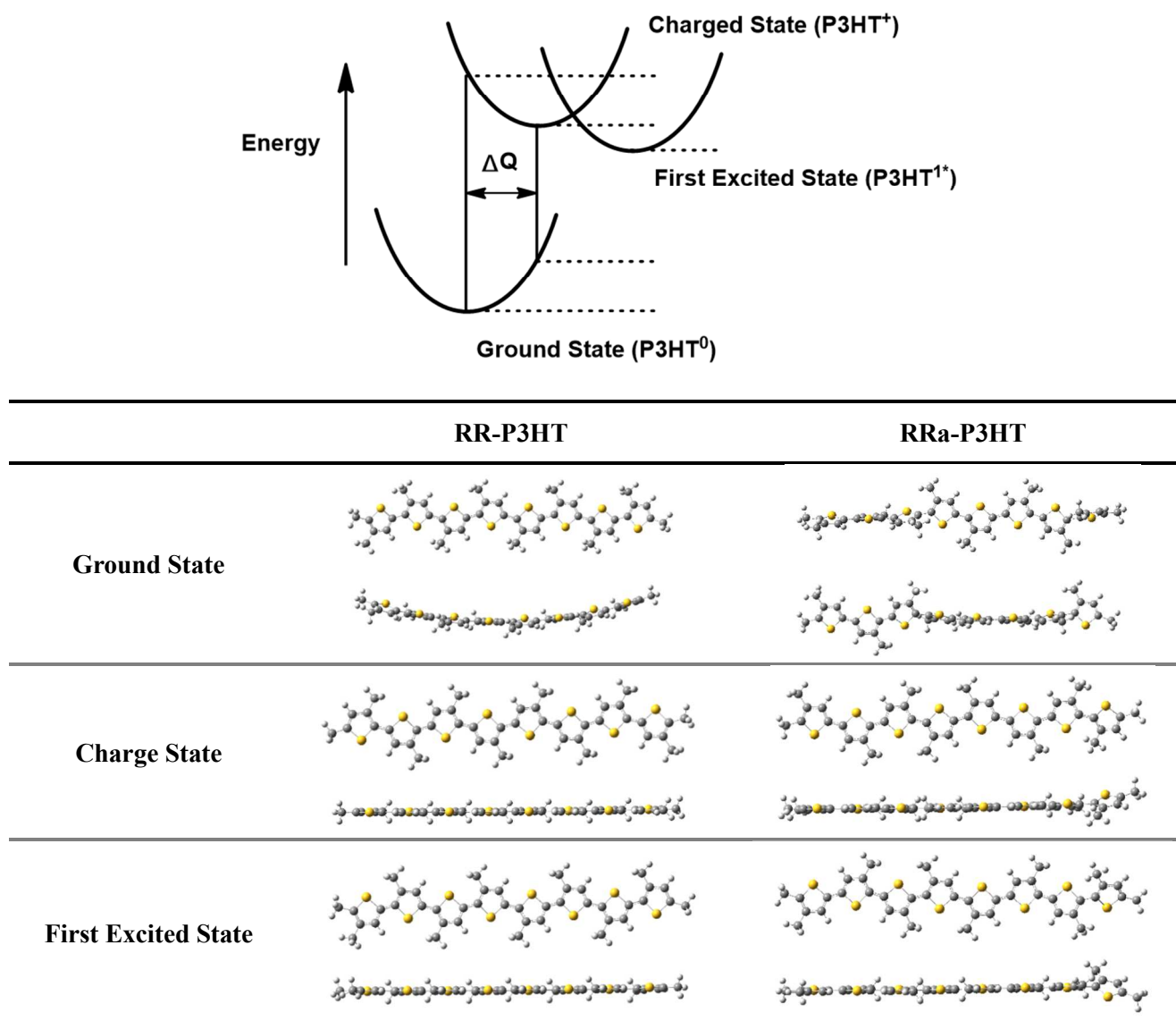


Figure S1. Optimized molecular structures (B3LYP/6-31G*) of ground, charged and first excited states of RR- and RRa-P3HT.

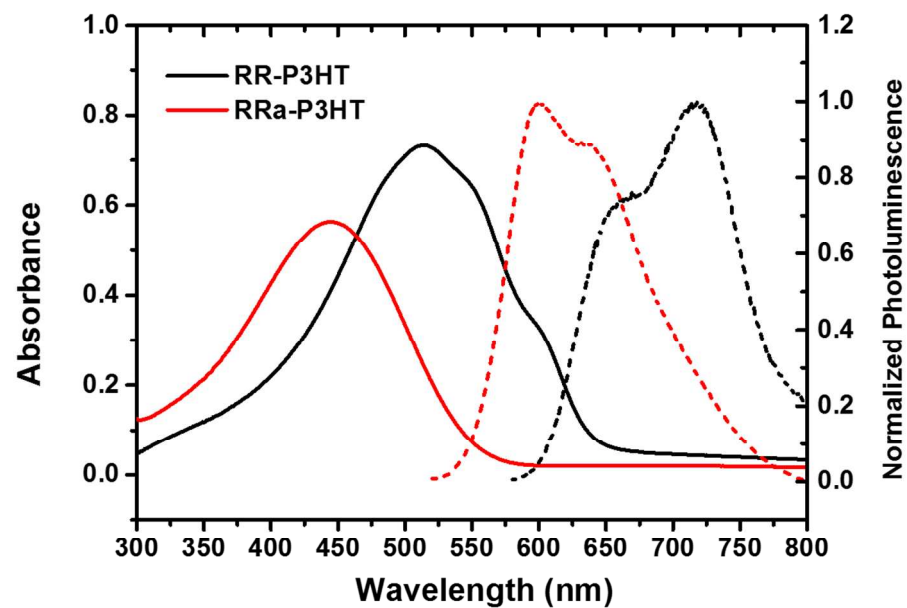


Figure S2. Absorption (solid line) and normalized photoluminescence spectra (dashed line) of RR- and RRa-P3HT. The pronounced red-shift of absorption and photoluminescence spectra of RR-P3HT compared to RRa-P3HT is a clear indication of the longer conjugation length of RR-P3HT induced by the ordered side chains.

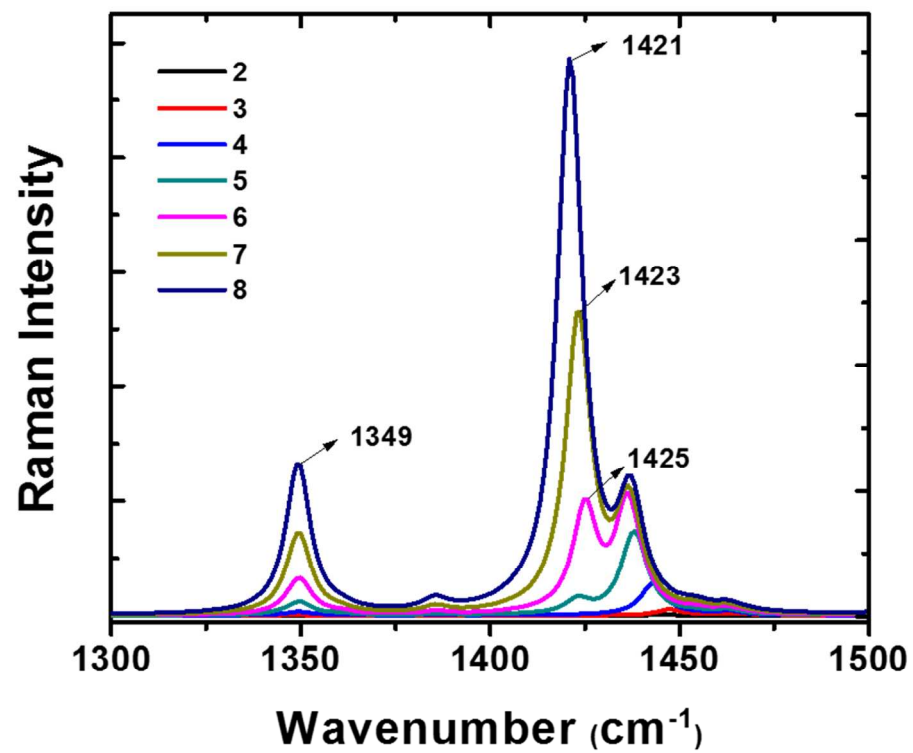
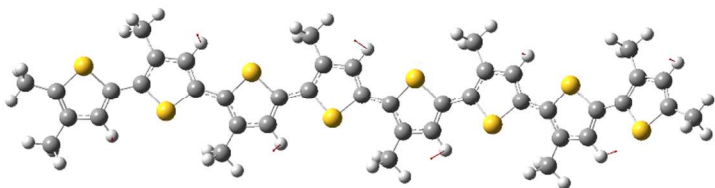
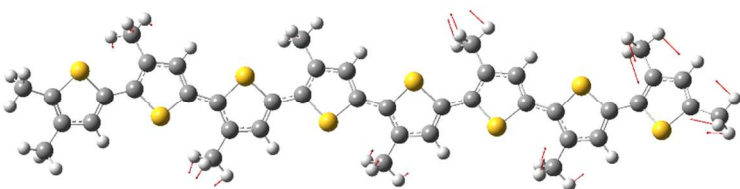


Figure S3. Calculated Raman spectra (B3LYP/6-31G*) of RR-P3HT with repeated units from 2 to 8.

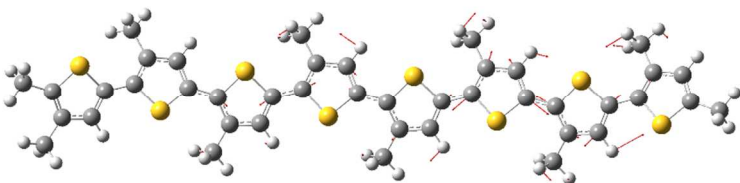
RR-P3HT



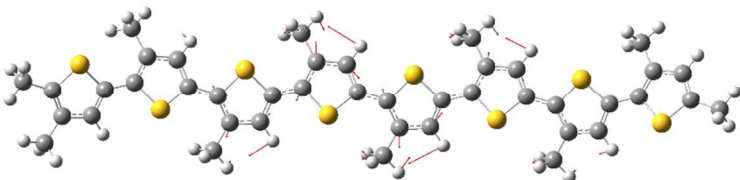
814 cm⁻¹



1386 cm⁻¹

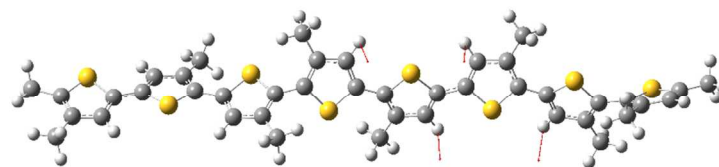


1426 cm⁻¹

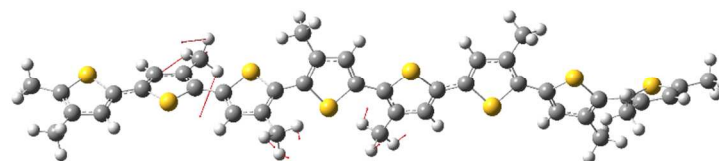


1499 cm⁻¹

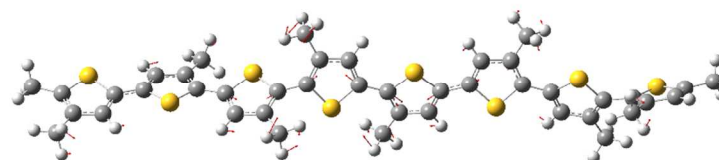
RRa-P3HT



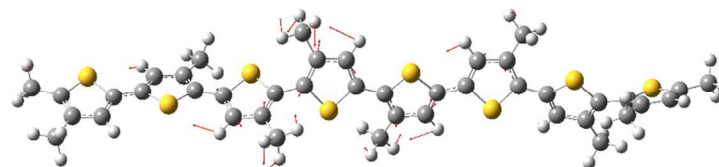
812 cm⁻¹



1387 cm⁻¹



1442 cm⁻¹



1510 cm⁻¹

Figure S4. B3LYP/6-31G* eigenvectors of vibrational modes for ground states of RR- and RRa-P3HT.

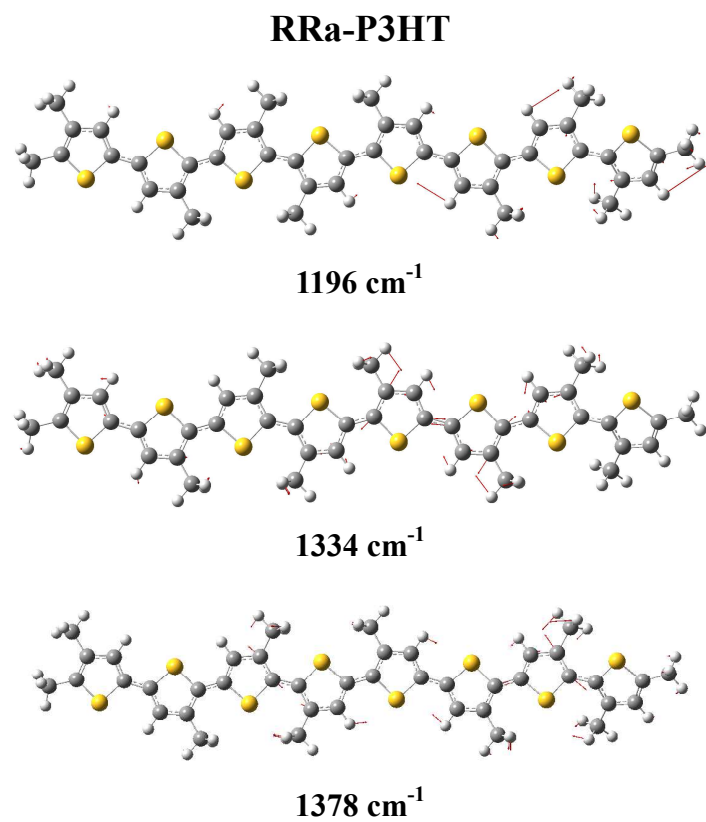
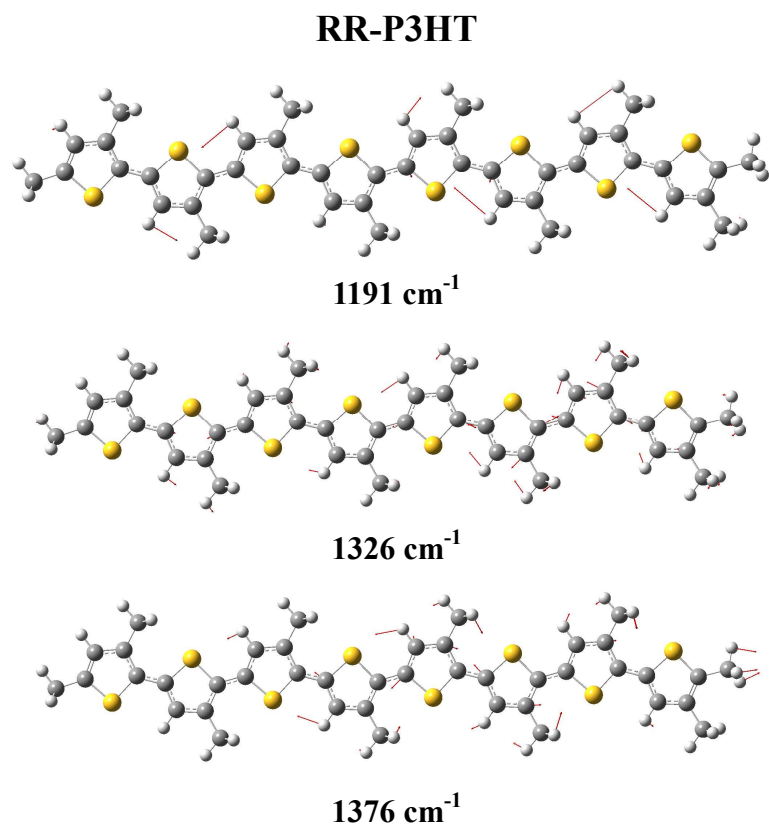
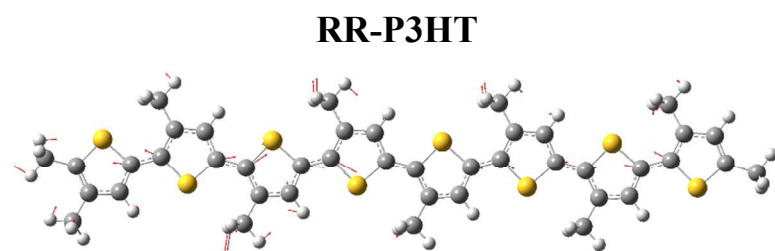
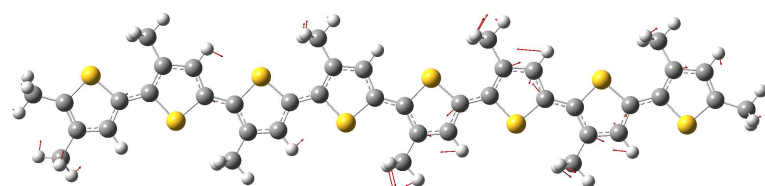


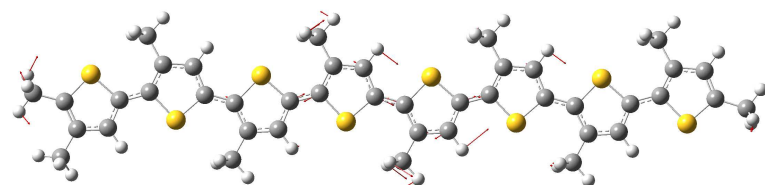
Figure S5. B3LYP/6-31G* eigenvectors of vibrational modes for polaron states (P3HT⁺) of RR- and RRa-P3HT.



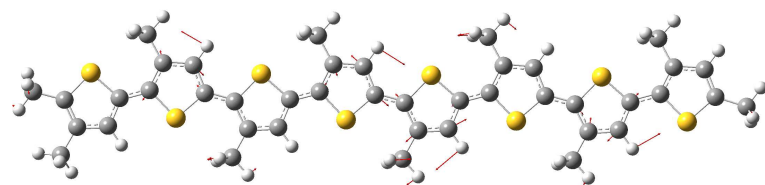
813 cm⁻¹



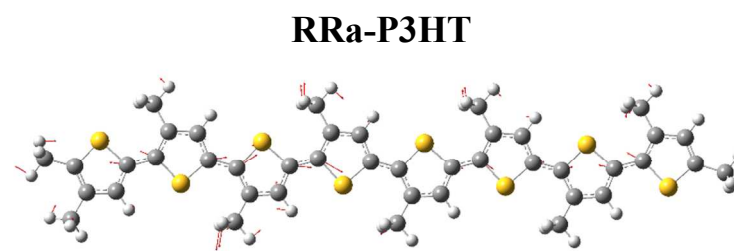
1354 cm⁻¹



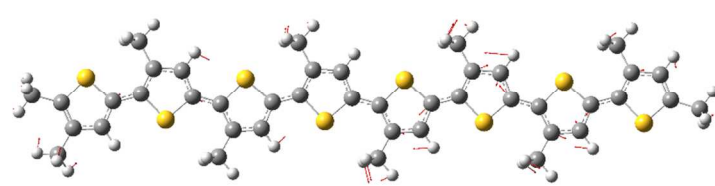
1446 cm⁻¹



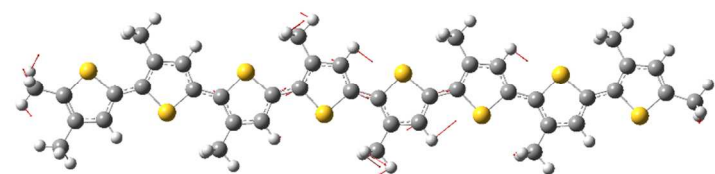
1486 cm⁻¹



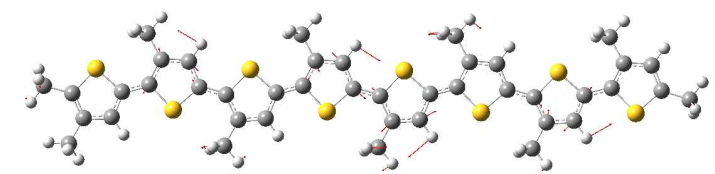
811 cm⁻¹



1363 cm⁻¹



1448 cm⁻¹



1500 cm⁻¹

Figure S6. B3LYP/6-31G* eigenvectors of vibrational modes for singlet excited states of RR- and RRa-P3HT.