

## Supporting Information of JP074784f

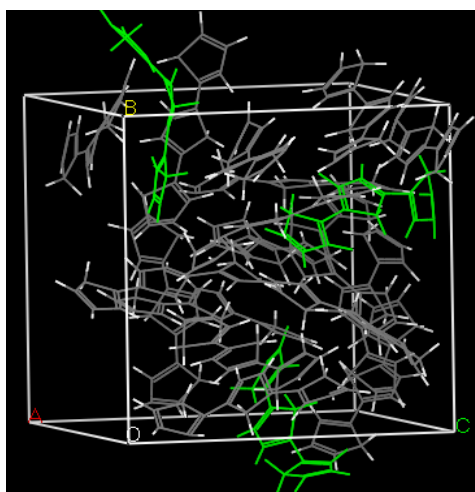
### “Inter-chain Impacts on Electronic Structures of Heterocyclic Oligomers and Polymers Containing Group 14, 15, and 16 Heteroatoms: Quantum Chemical Calculations in Combination with Molecular Dynamics Simulations”

by Guiling Zhang,<sup>†,‡</sup> Jing Ma,<sup>†,\*</sup> and Jin Wen

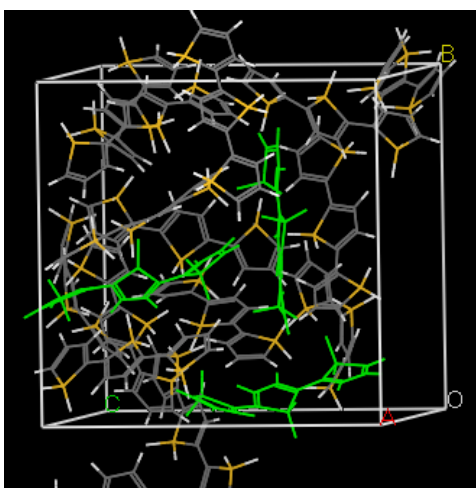
**Figure S1.** Snapshots of oligoheterocycle systems, **1-6** ( $n=3/2$ ), from MD simulations at 200 ps. The green-colored chains enable us to easily perceive the chain distortions.

**Figure S2.** The statistic distribution of effective conjugated length (*ECL*) for short-length ( $n=3/2$ ) oligoheterocycle systems by MD/PCFF simulations.

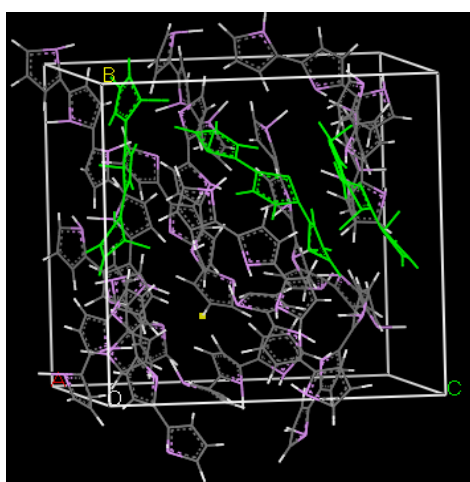
**Figure S3.** Radial distribution functions  $f(r)$  of distances between two centers of mass of two thiophene rings in different chains of various packing systems within the inter-chain distance of 4.0 Å.



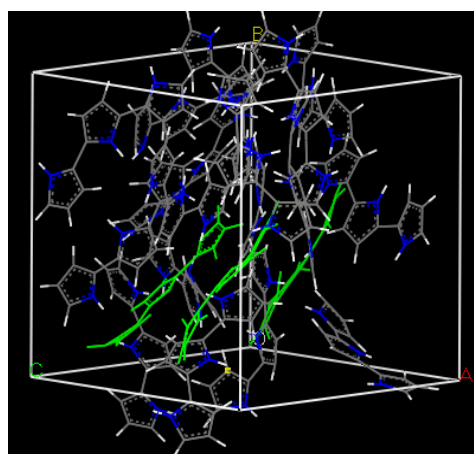
*nCp* ( $n=3/2$ )



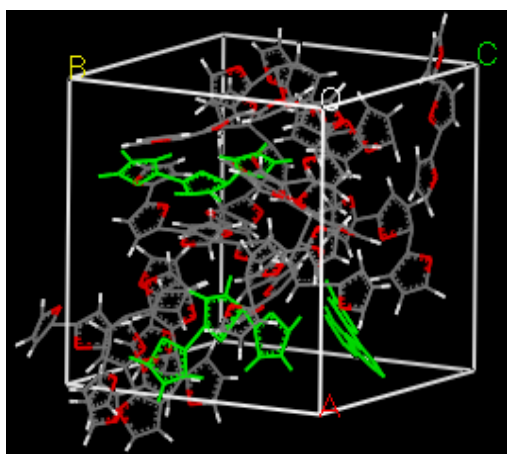
*nSi* ( $n=3/2$ )



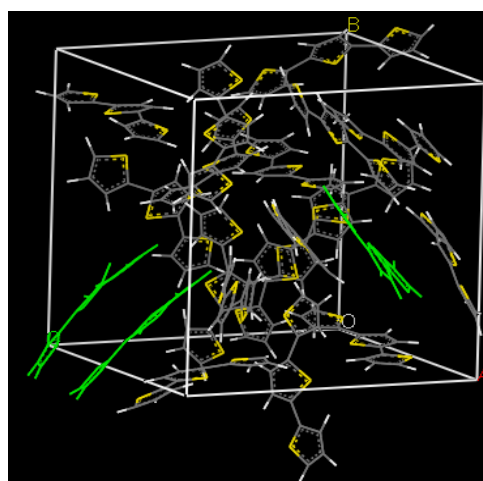
*nPy* ( $n=3/2$ )



*nPh* ( $n=3/2$ )

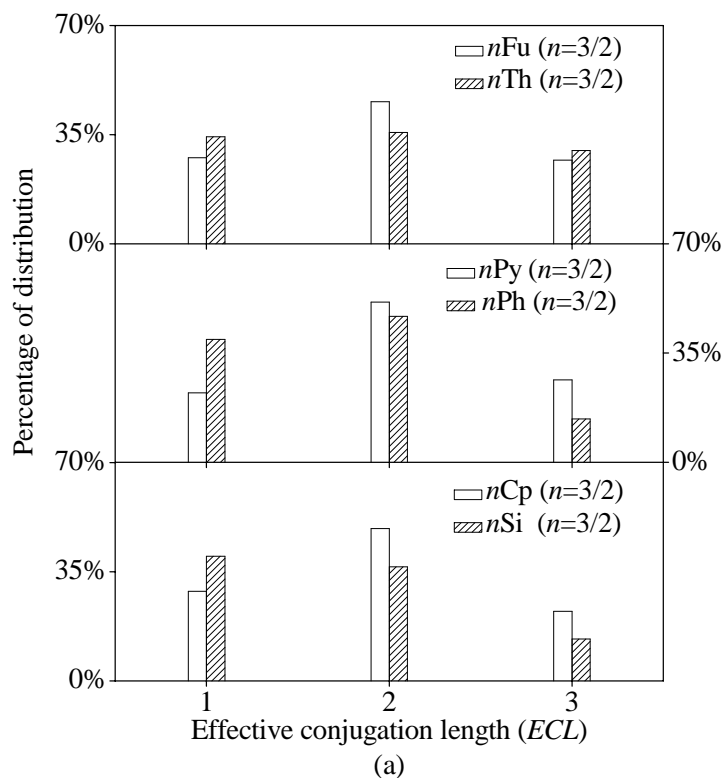


*nFu* ( $n=3/2$ )

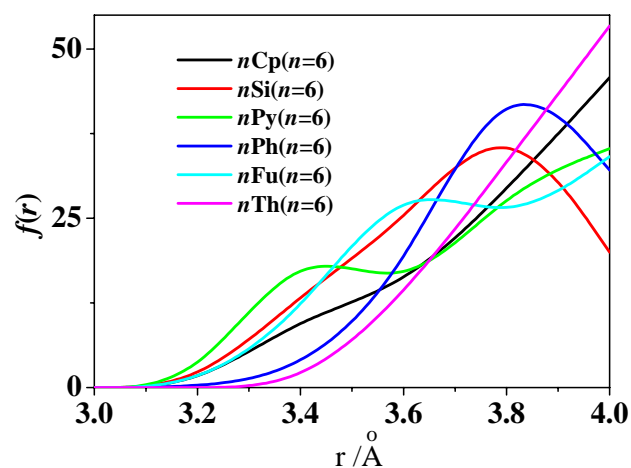


*nTh* ( $n=3/2$ )

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