Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Control of Molecular Orientations of Poly(3-hexylthiophene) on Self-Assembled Monolayers: Molecular Dynamics Simulations

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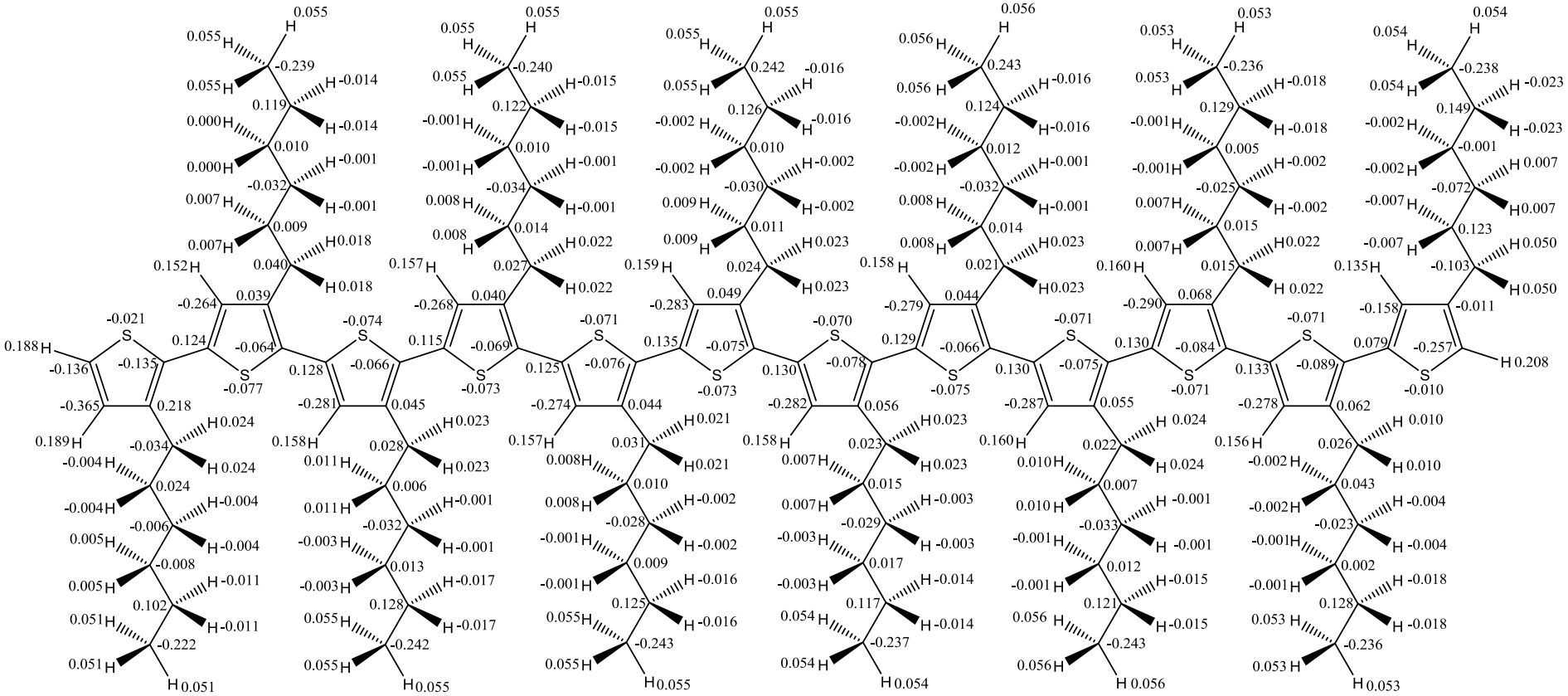
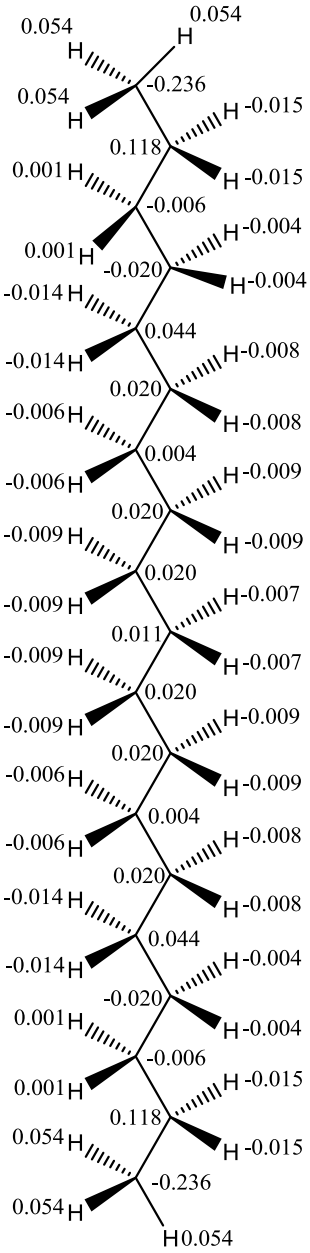
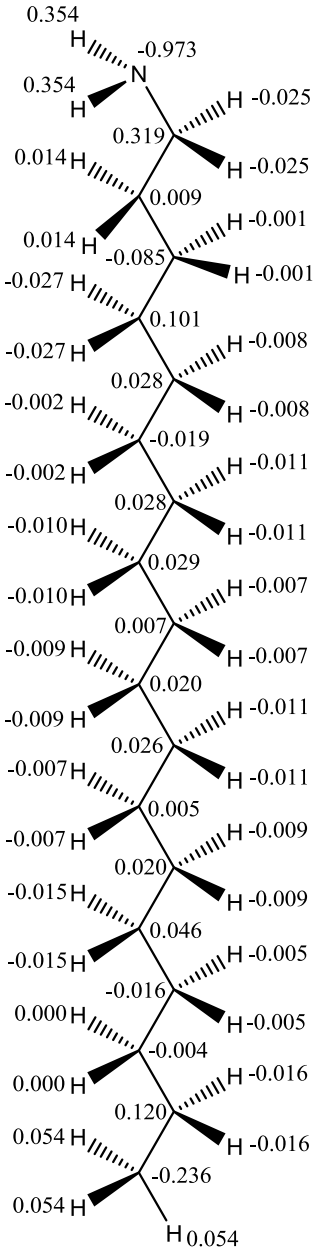


(a)

Figure S1. Atomic charges for the (a) O3HT, (b) liner alkane, and (c) NH_2-terminated molecule used in MD simulations. For the evaluation method of the atomic charges, see Sec. 2 in the main text.



(b)



(c)

Figure S1. Continued.

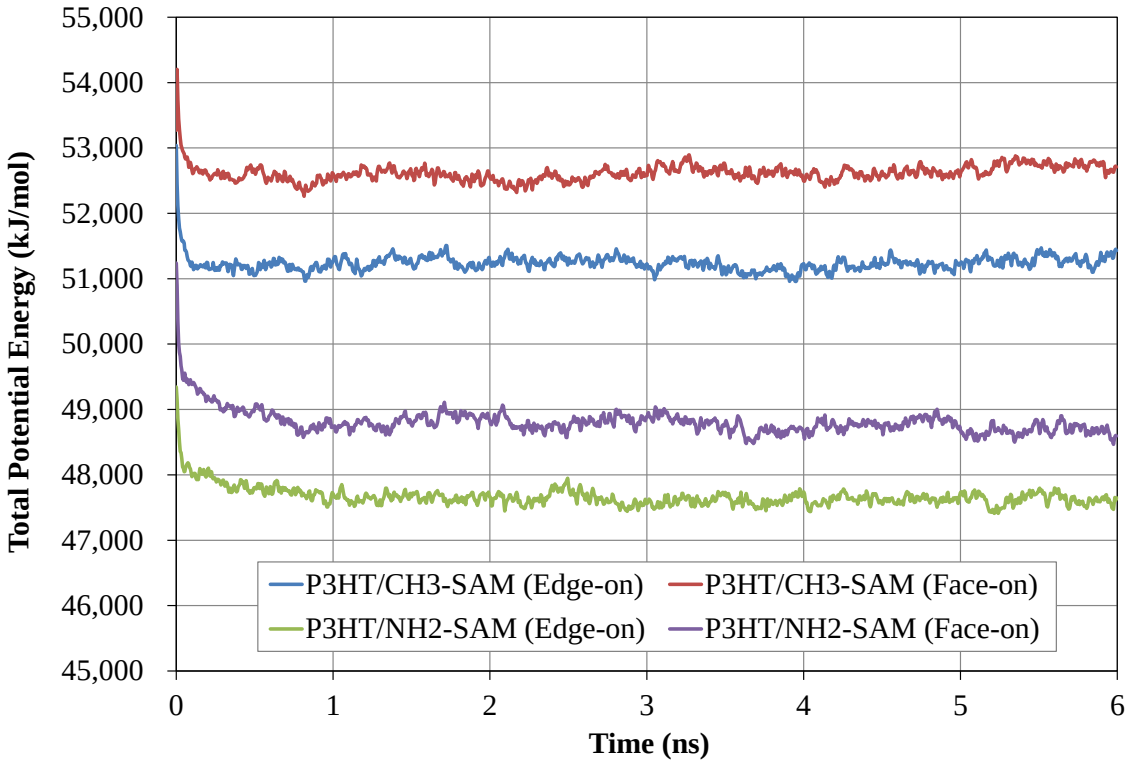


Figure S2. Total potential energies as a function of simulation time for the model systems of P3HT on the CH_3-terminated and NH_2-terminated SAMs.

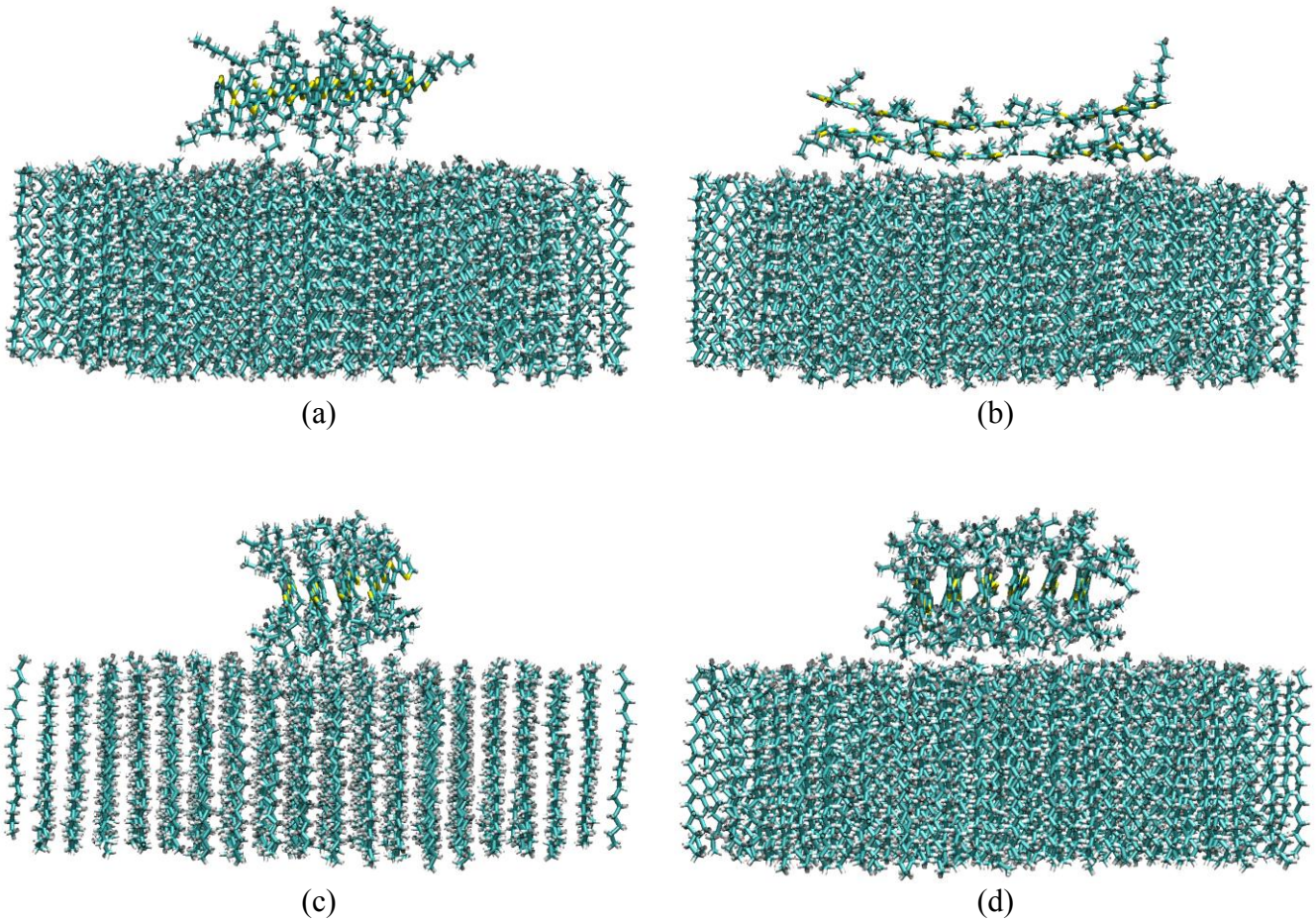
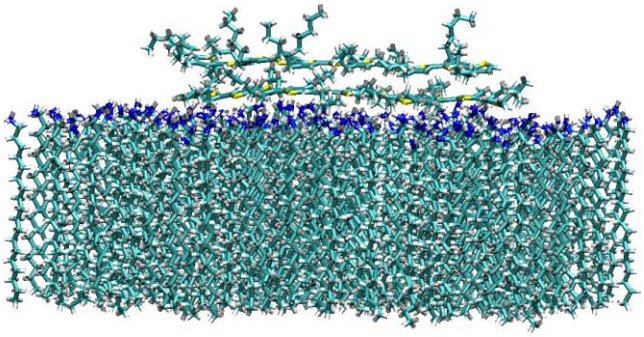
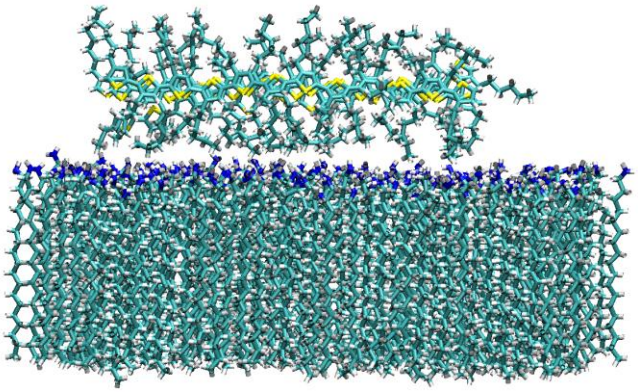


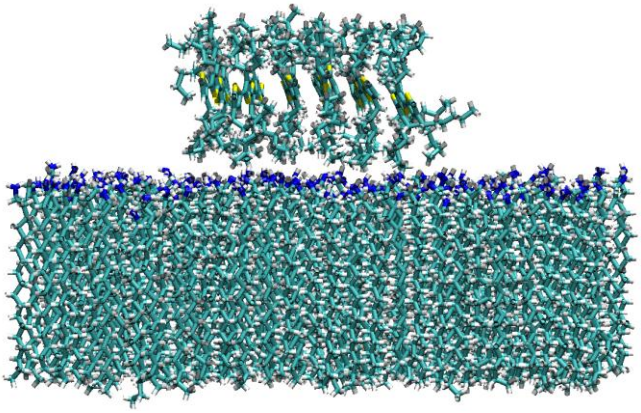
Figure S3. MD snapshots of simulation for the systems with a limited number of O3HT molecules. In (a)-(d), the SAM system is the CH_3-terminated SAM and the number of stacked O3HT molecules are two (a and b), four (c), and six (d). Panels (e)-(g) show the systems of two-, four-, and six-stacked O3HTs and the NH_2-terminated SAM, respectively. The simulation time is at 1.2 ns for (a) and 4 ns for the other panels. The O3HT takes the face-on orientation in (b) and (e) and the edge-on orientation in the other panels.



(e)



(f)



(g)

Figure S3. Continued.