Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Molecular Dynamics Simulation of α-Unsubstituted Oligo-thiophenes: Dependence of their High-Temperature Liquid-Crystalline Phase Behaviour on Molecular Length

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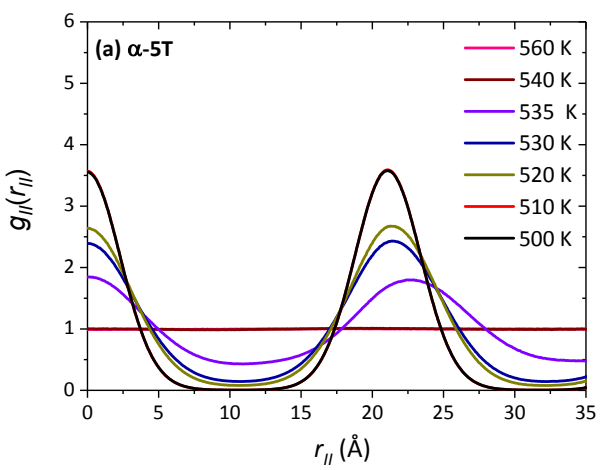
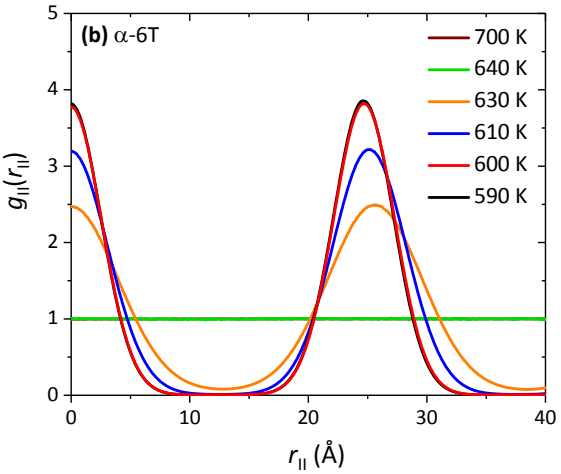
Electronic Supplementary Information (ESI)

The supplementary information file is organised as follows: in Section 1, the calculated pair correlation functions of α-unsubstituted oligo-thiophenes with number of thiophene rings n = 5 - 8 (α-5T, α-7T, α-6T and α-8T) are presented. The atomistic snapshots of the crystal phases from our MD simulations are displayed in Section 2.

1. Calculated pair correlation functions of α-unsubstituted oligo-thiophenes.

1.1 Longitudinal $g_{II}(r_{II})$ pair correlation function





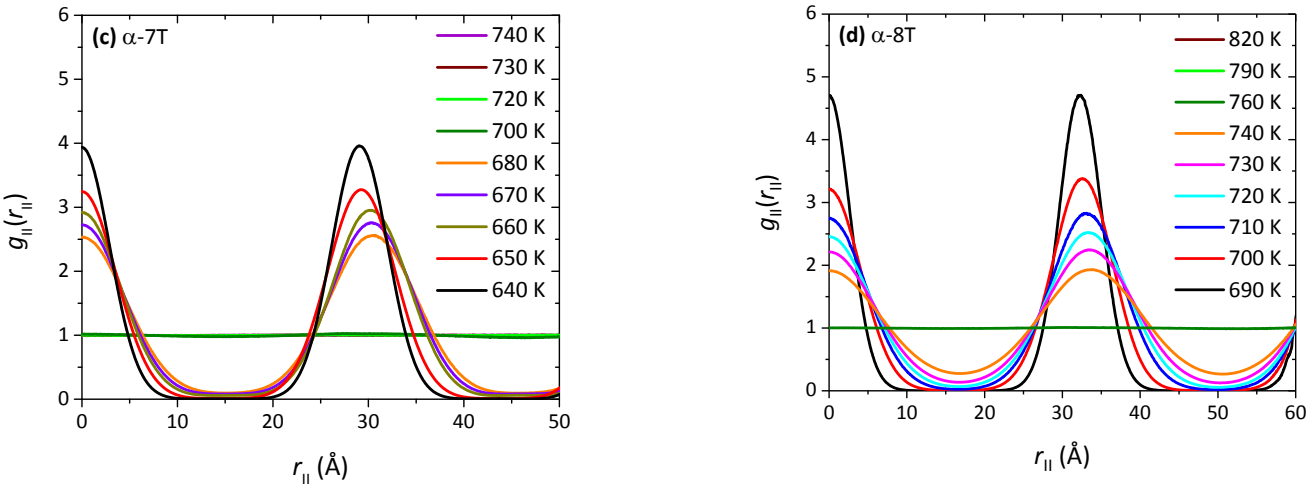
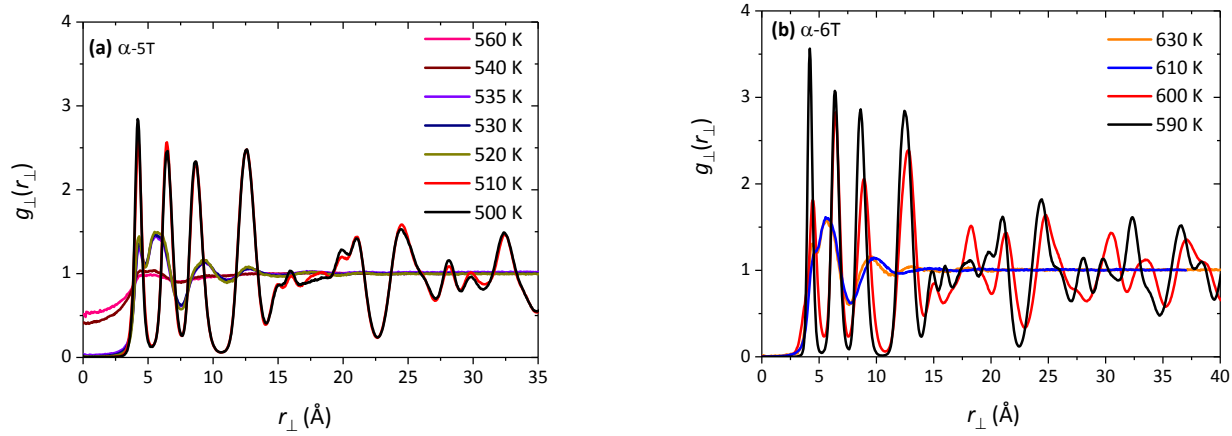


Fig. S1 Longitudinal pair correlation functions of: (a) α-5T, (b) α-6T, (c) α-7T, and (d) α-8T at various temperatures (and P = 1 atm) as predicted from our MD simulations.

1.2 Perpendicular $g_{\perp}(r_{\perp})$ pair correlation function



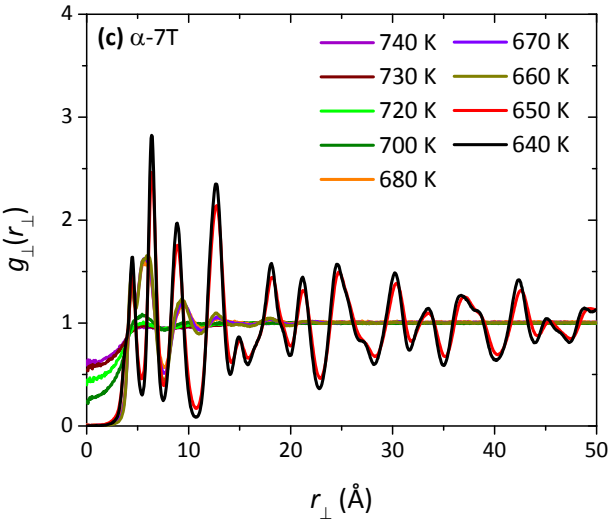
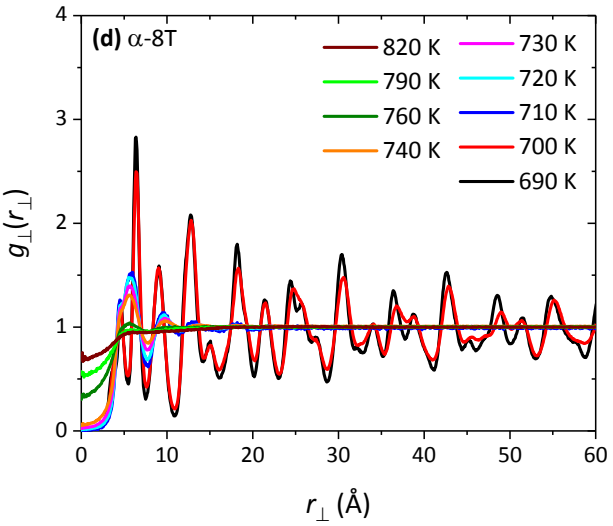
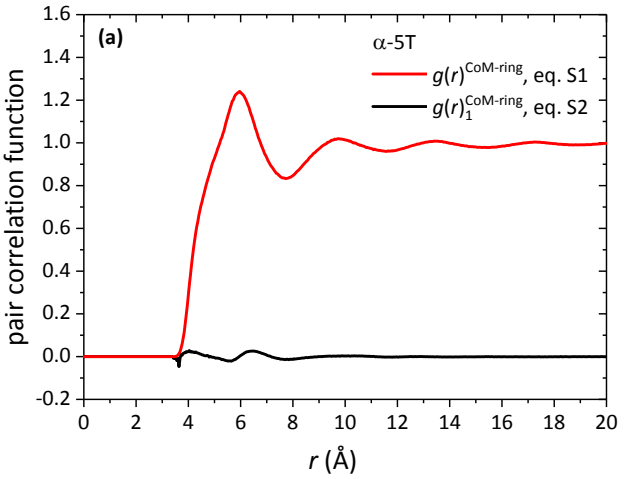
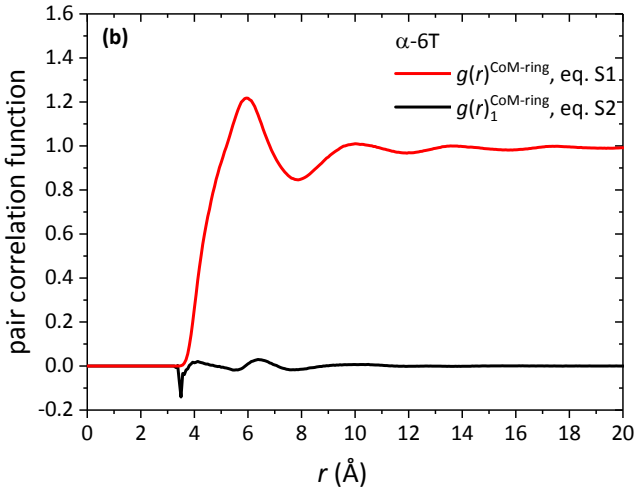


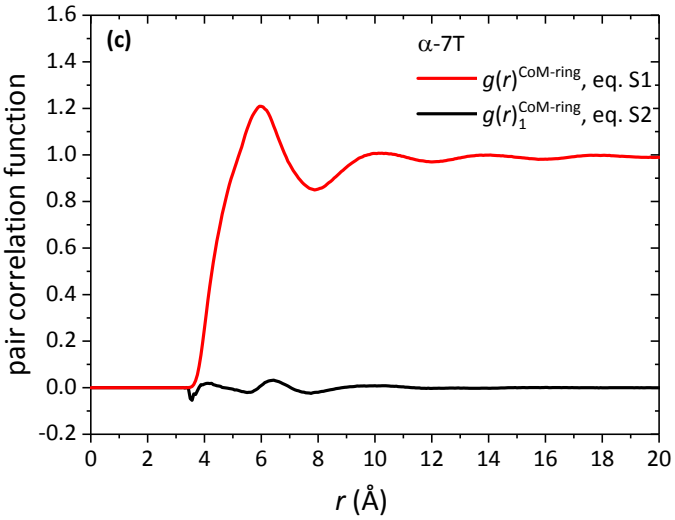
Fig. S2 Perpendicular pair correlation functions of: (a) α-5T, (b) α-6T, (c) α-7T and (d) α-8T at various temperatures (and P = 1 atm) as predicted from our MD simulations.



1.3 $g^{\text{CoM-ring}}(r)$ and $g_1^{\text{CoM-ring}}(r)$ pair correlation functions







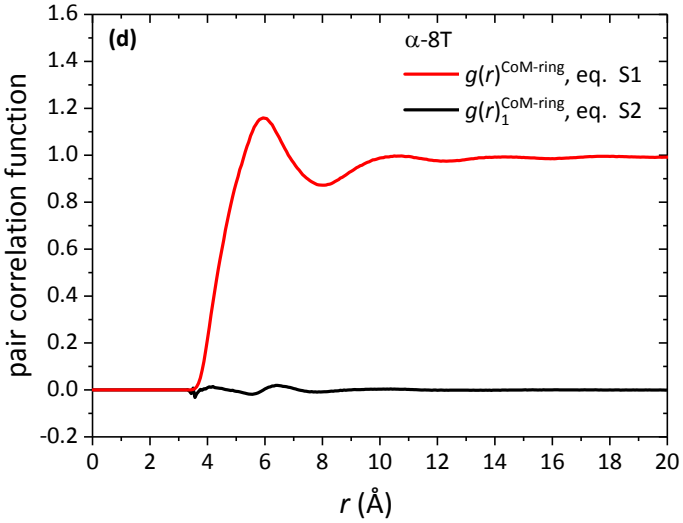
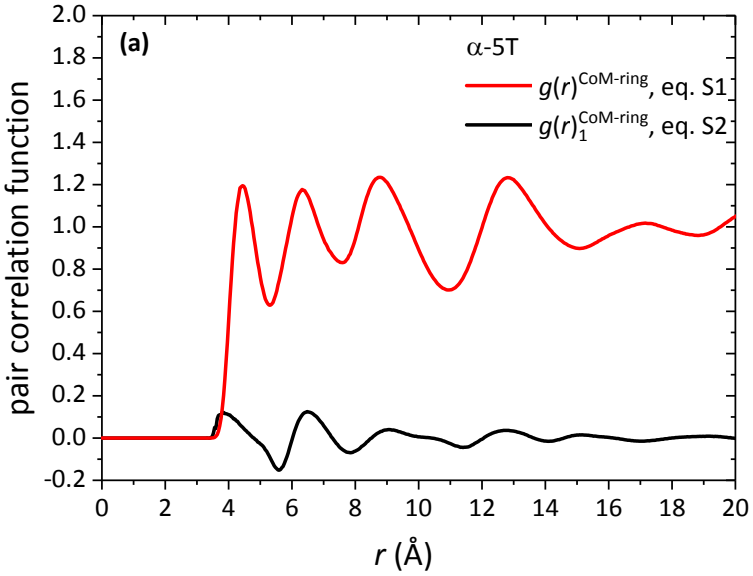
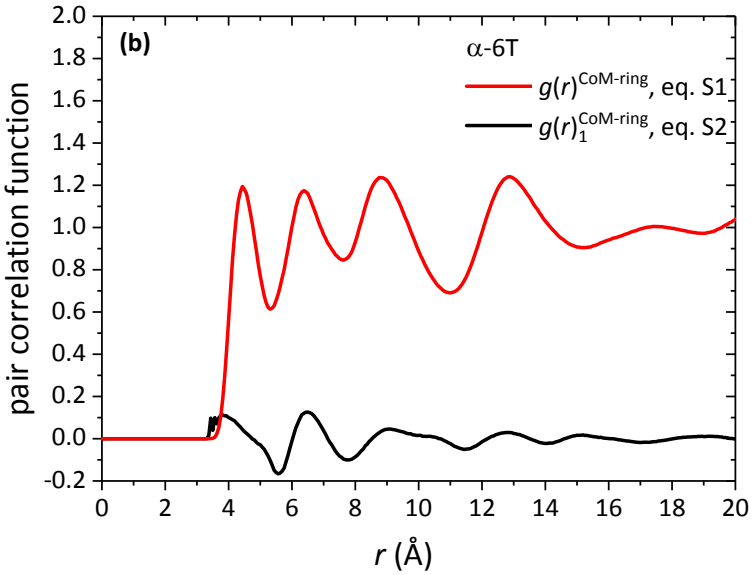


Fig. S3 Plots of the $g^{\text{CoM-ring}}(r)$ and $g_1^{\text{CoM-ring}}(r)$ pair correlation functions corresponding to the smectic-A phases of: (a) α-5T, (b) α-6T, (c) α-7T and (d) α-8T, at T = 530 K, 620 K, 690 K, and 740 K, respectively, as obtained from our *NPT* MD simulations (P = 1 atm).


(a)
α-5T
$g(r)^{\text{CoM-ring}}$, eq. S1
$g(r)_1^{\text{CoM-ring}}$, eq. S2
pair correlation function
r (Å)


(b)
α-6T
$g(r)^{\text{CoM-ring}}$, eq. S1
$g(r)_1^{\text{CoM-ring}}$, eq. S2
pair correlation function
r (Å)

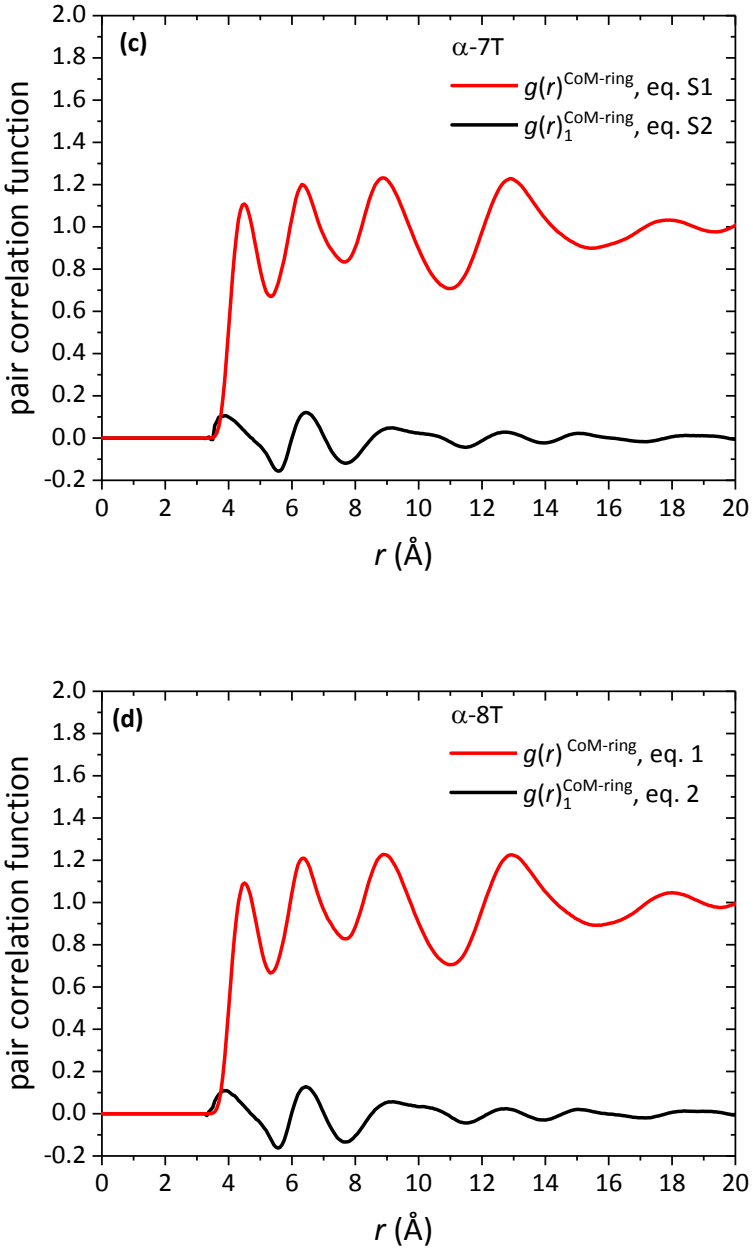


Fig. S4 Same as with Fig. S4 but for the corresponding crystal phases of α-5T, α-6T, α-7T and α-8T at T = 490 K, 590 K, 640 K and 690 K, respectively.

2. Snapshots of the crystal phases

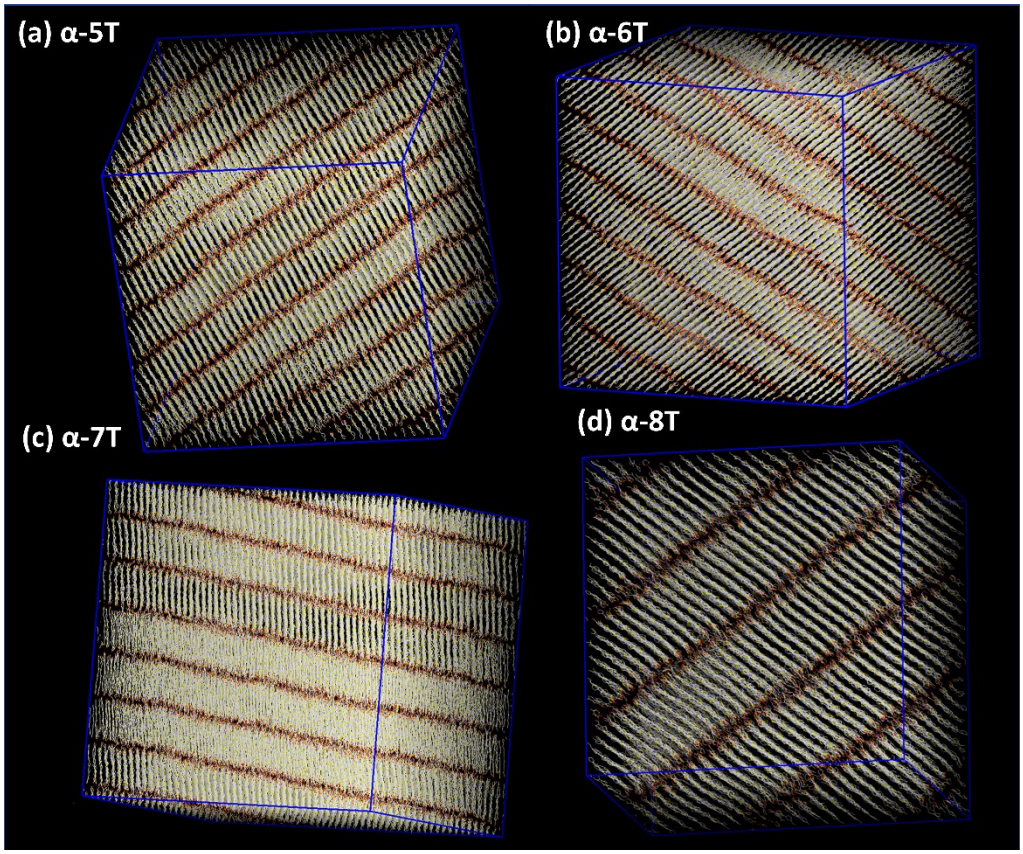


Fig. S5 Characteristic atomistic snapshots of the crystal phases of: (a) α-5T, (b) α-6T, (c) α-7T and (d) α-8T, at T = 490 K, 590 K, 640 K and 690 K, respectively, as obtained from our *NPT* MD simulations (P = 1 atm).