Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information: The Structure of Liquid Thiophene from Total Neutron Scattering

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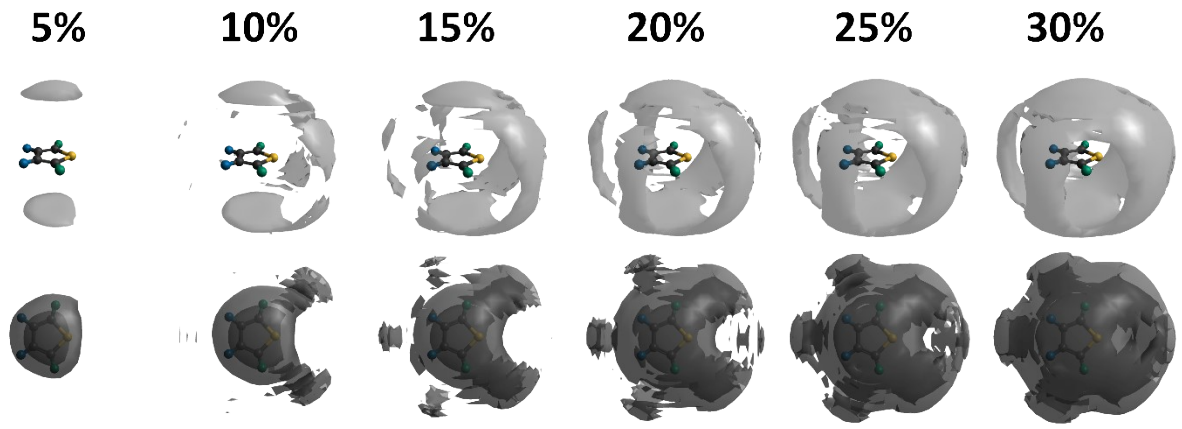

Figure S1. SDFs of CoR at increasing percentage most likely positions.

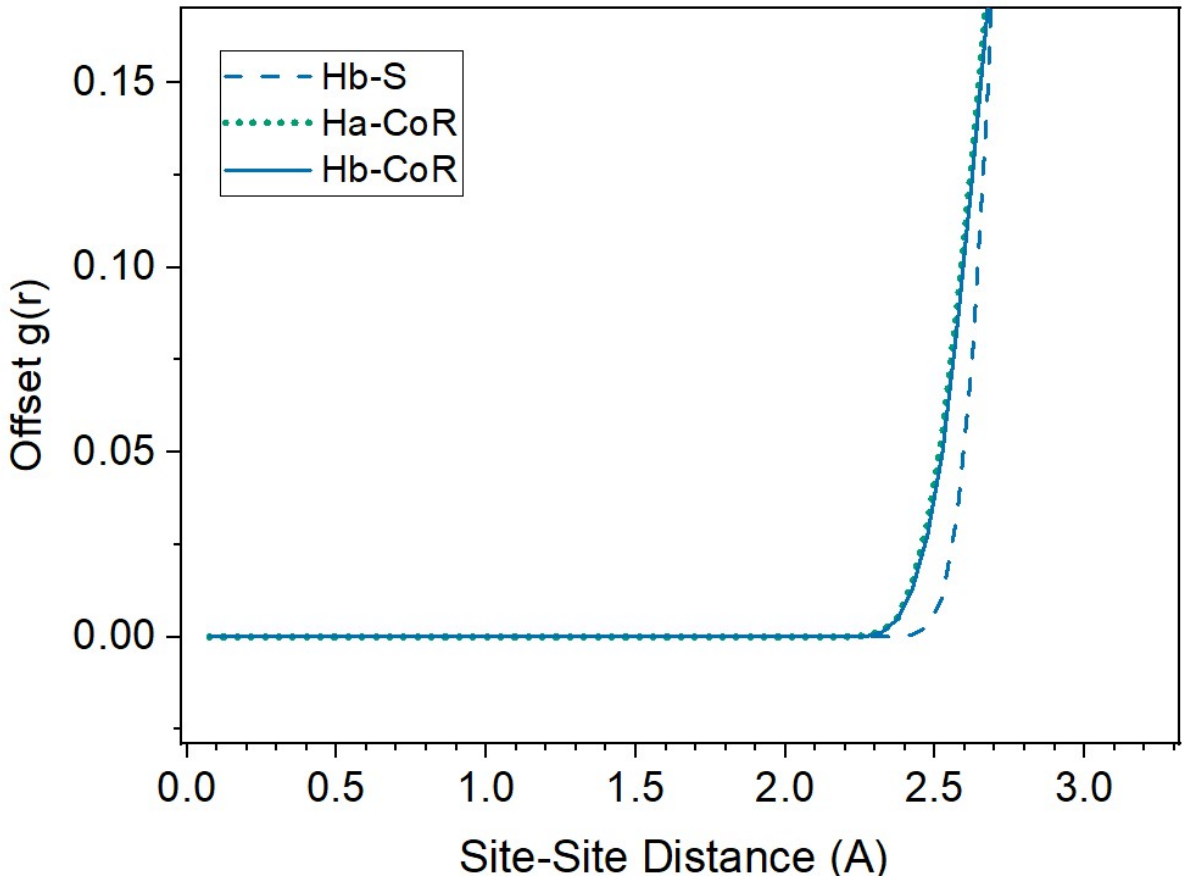

Figure S2. RDF of H_a/H_b -CoR and Hb-S at the peak onset, showing closest H-CoR interactions are at lower distances than the closest H-S interactions.

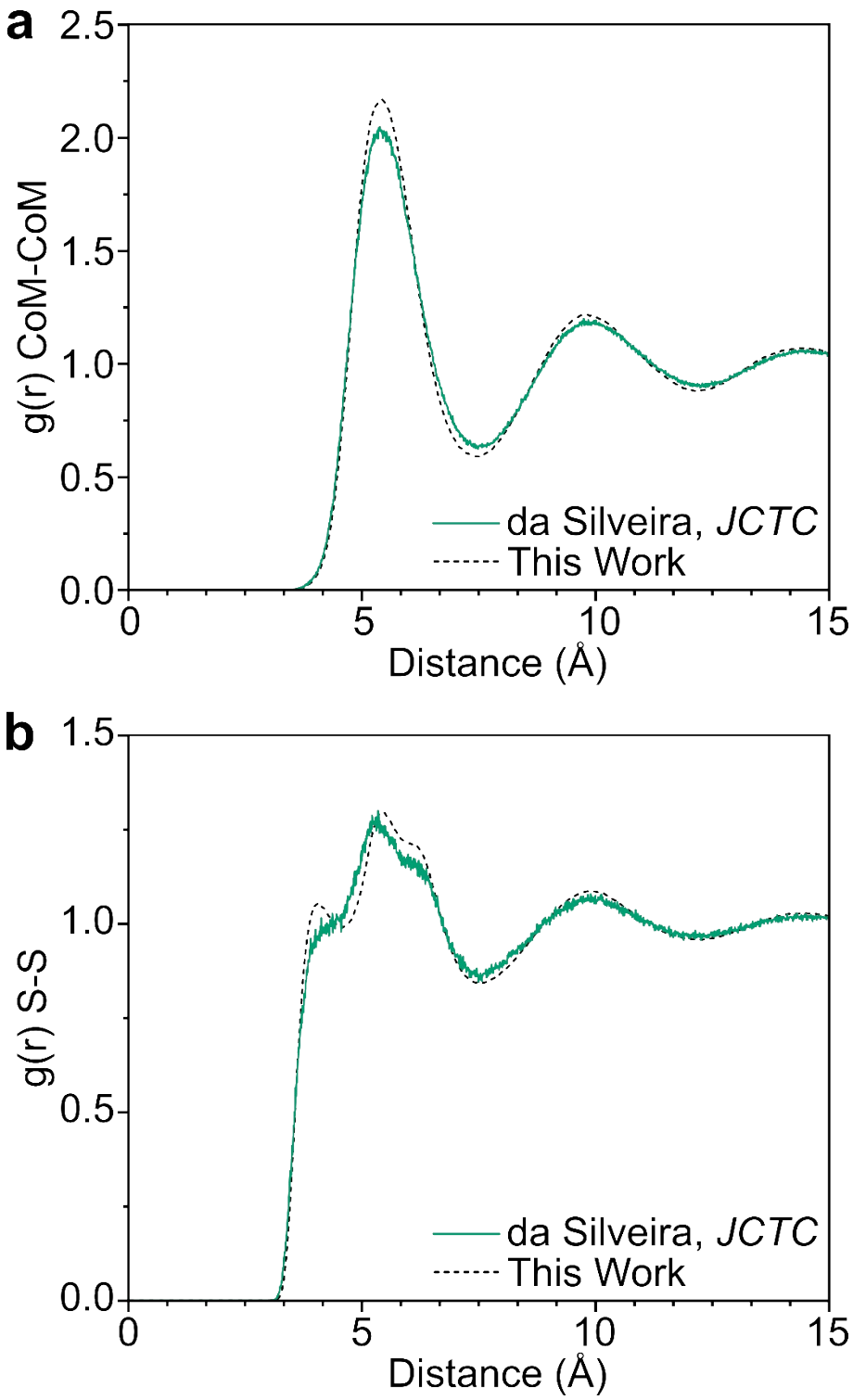

Figure S3. Comparison of radial distribution functions for liquid thiophene for (a) CoM-CoM and (b) S-S interactions, calculated from this work and from a DFT derived force-field in de Silveira *et al*., *Journal of Chemical Theory and Computation,* **2018**, *14*, 4884-4900.

Table S1. Table of input parameters

Atom	Cartesian Coordinates (Å)			Charge	L. J. Seed Potentials	
	X	Y	Z	(e)	ε	σ
C_ai	1.516	1.000	1.278	-0.2488	0.29288	3.55
$C_a$ii	-0.941	1.000	1.278	-0.2473	0.29288	3.55
C_bi	1.000	1.000	0.000	-0.1551	0.29288	3.55
$C_b$ii	-0.425	1.000	0.000	-0.1548	0.29288	3.55
S	0.290	1.000	2.467	+0.0730	1.48532	3.60
H_ai	2.556	1.001	1.572	+0.1908	0.12552	2.42
$H_a$ii	-1.981	0.999	1.572	+0.1908	0.12552	2.42
H_bi	1.614	1.001	-0.892	+0.1756	0.12552	2.42
$H_b$ii	-1.040	1.001	-0.892	+0.1756	0.12552	2.42
CoR	0.288	1.000	1.005			
CoM	0.288	1.000	1.321			