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

Supporting Information

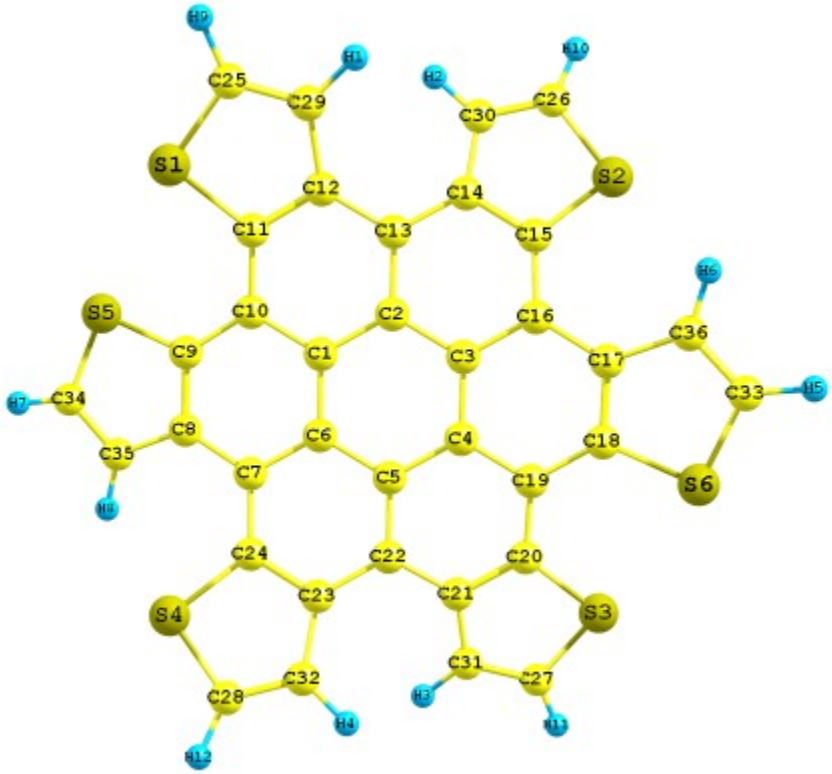
Forth-Back Oscillated Charge Carrier Motion in Dynamically Disordered Hexathienocoronene molecules: A Theoretical Study

K. Navamani and K. Senthilkumar*

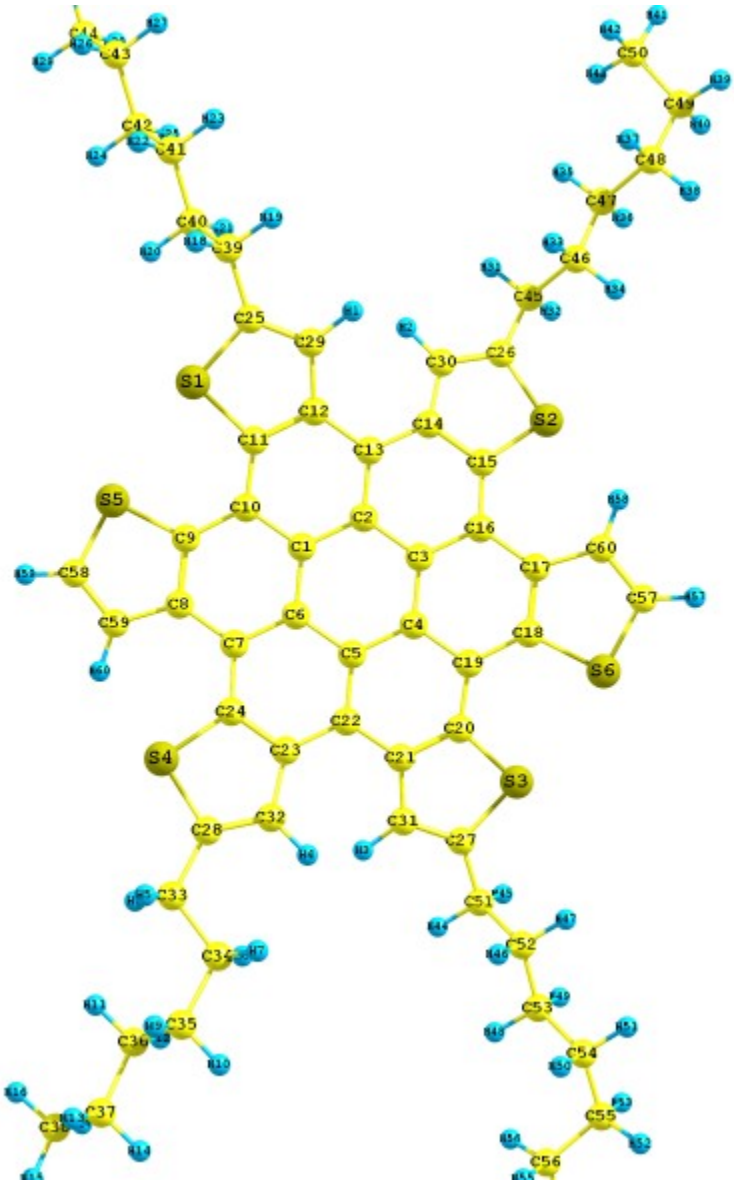
Department of Physics, Bharathiar University, Coimbatore-641 046

*Corresponding author: ksenthil@buc.edu.in

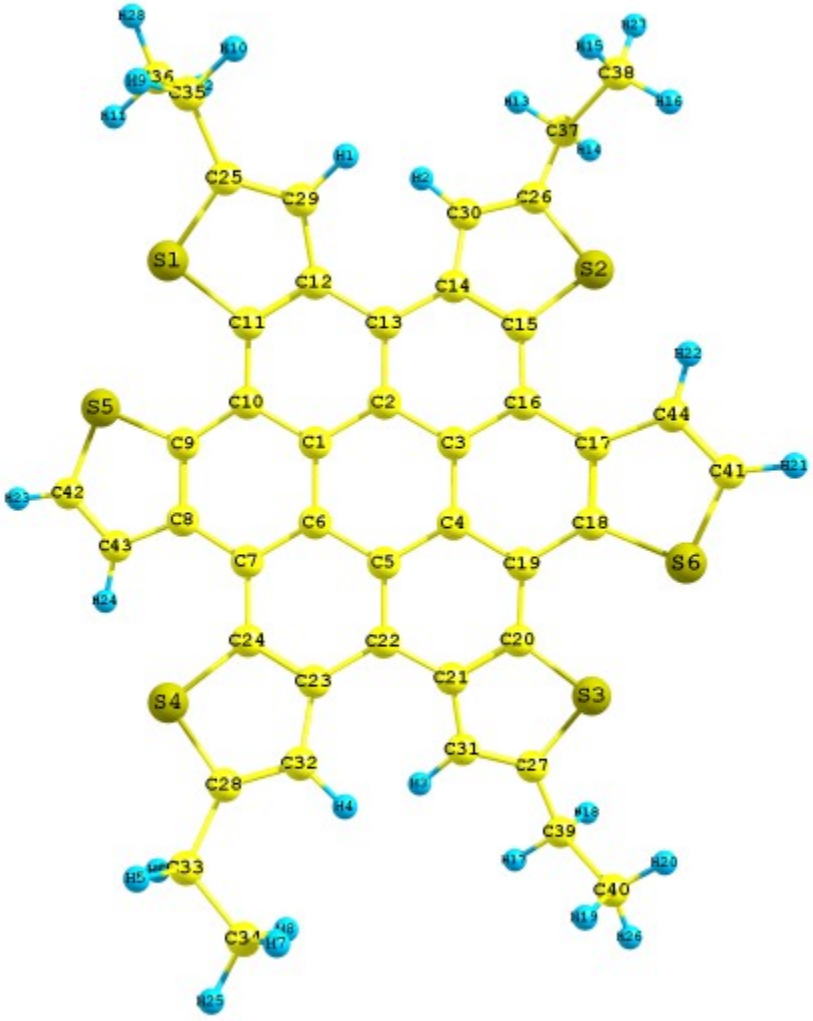
Fig. S1 Optimized structures of unsubstituted hexathienocoronene (HTC-a), hexyl substituted hexathienocoronene (HTC-b), ethyl substituted hexathienocoronene (HTC-c) molecules



HTC-a

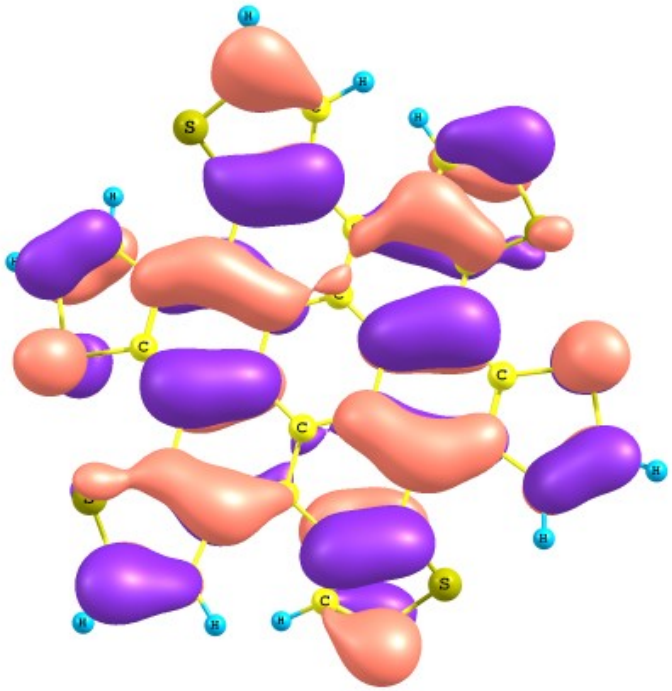


HTC-b

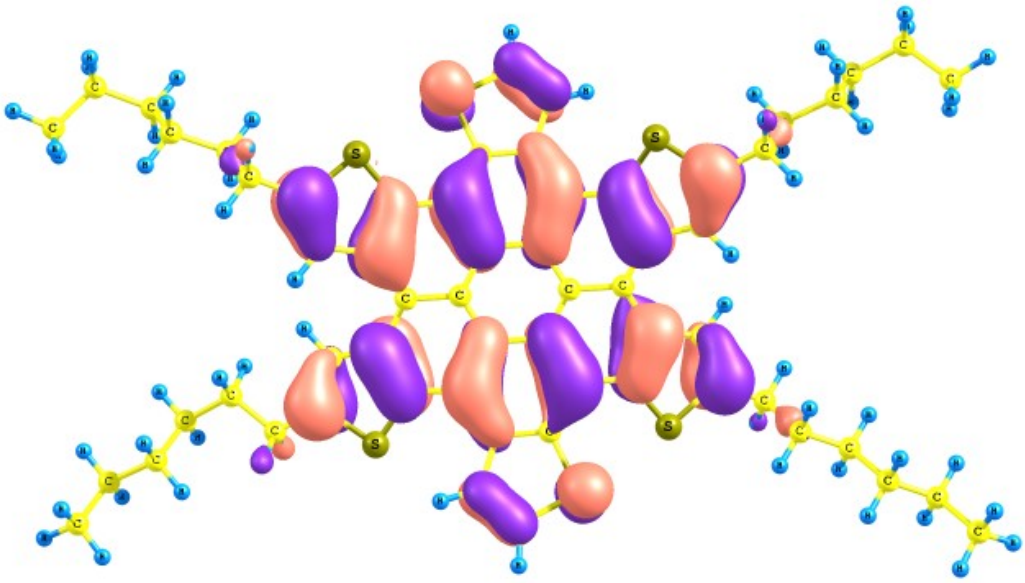

S1
S2
S3
S4
S5
S6
C1
C2
C3
C4
C5
C6
C7
C8
C9
C10
C11
C12
C13
C14
C15
C16
C17
C18
C19
C20
C21
C22
C23
C24
C25
C26
C27
C28
C29
C30
C31
C32
C33
C34
C35
C36
C37
C38
C39
C40
C41
C42
C43
C44

HTC-c

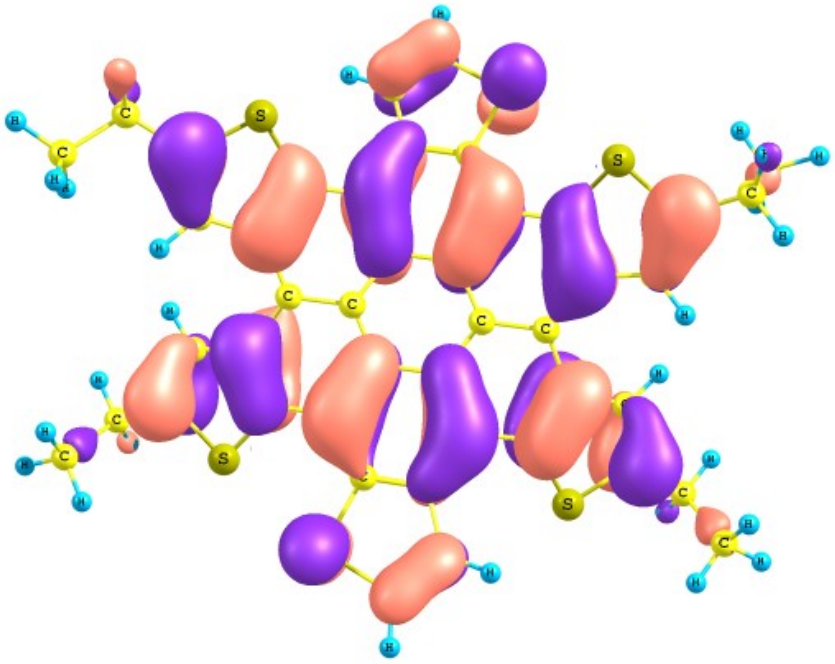
Fig. S2 The density plot of Highest Occupied Molecular Orbital (HOMO) of the studied molecules HTC-a, HTC-b and HTC-c



HTC-a

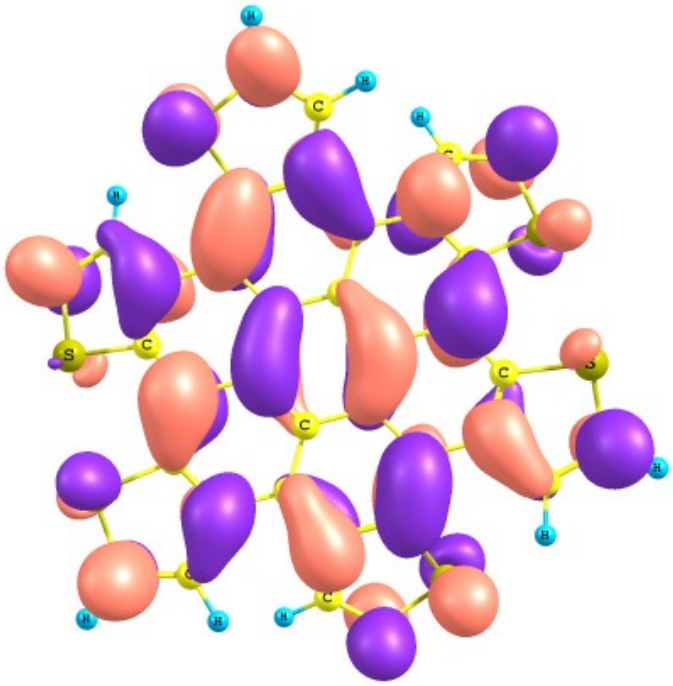


HTC-b

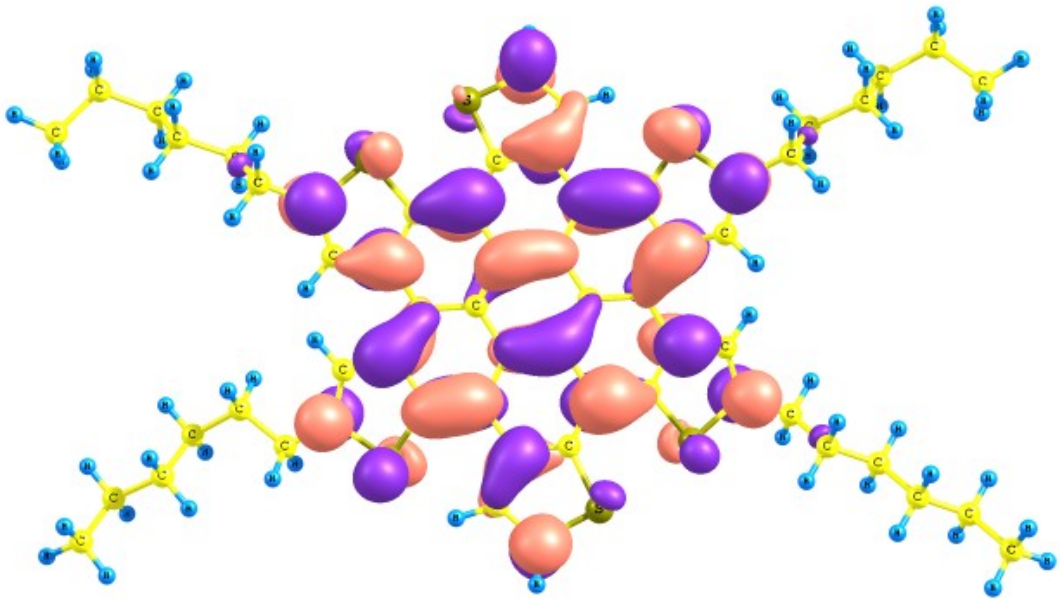


HTC-c

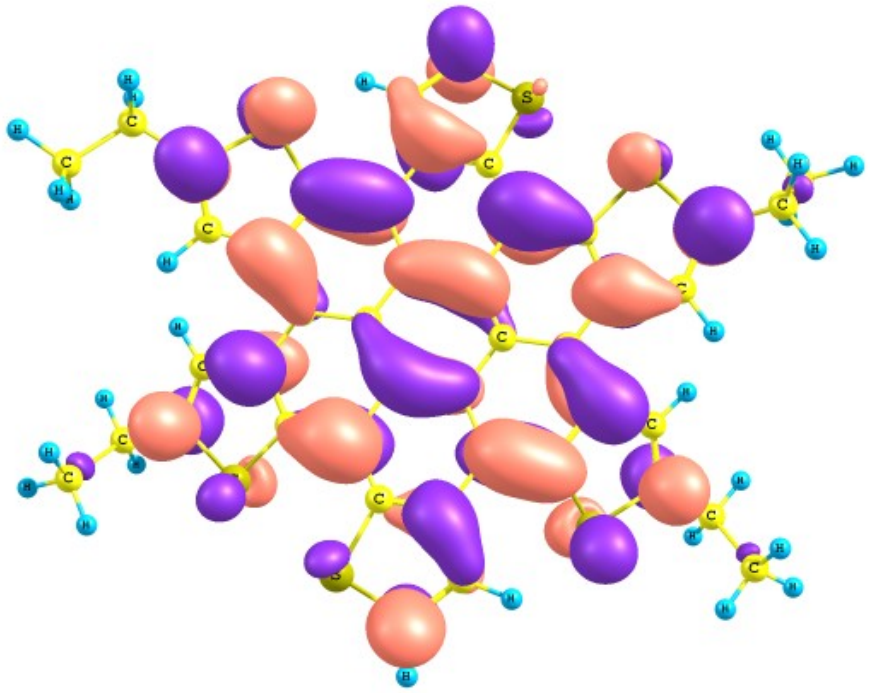
Fig. S3 The density plot of Lowest Unoccupied Molecular Orbital (LUMO) of the studied molecules HTC-a, HTC-b and HTC-c



HTC-a



HTC-b



HTC-c

Fig. S4 The plot between the number of occurrence, potential energy with respect to stacking angle calculation from molecular dynamics simulation for unsubstituted HTC (HTC-a) molecule

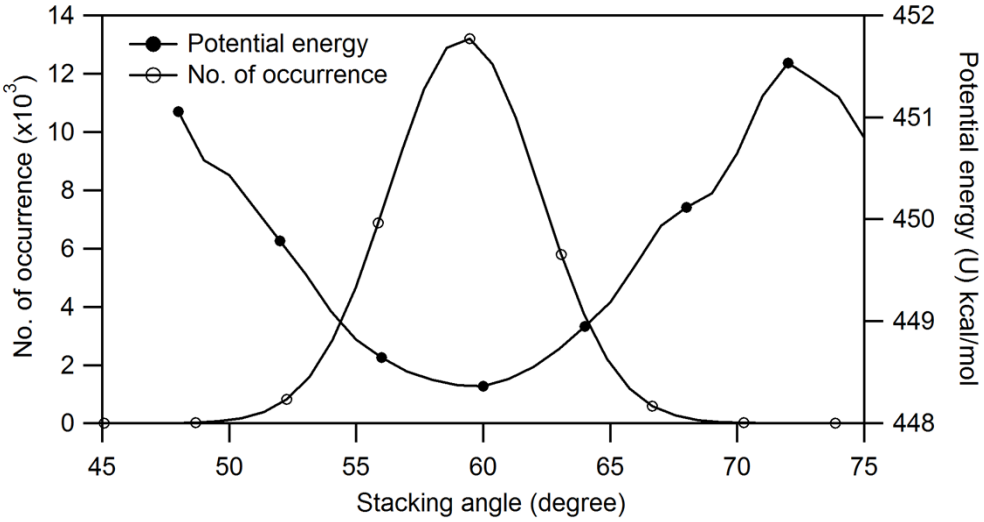


Table S1. The effective charge transfer integral (J_{eff}) at different stacking angle (θ) for hole and electron transport in the studied HTC-a, HTC-b and HTC-c molecules.

Stacking angle *(θ)* in degree	J_{eff} in eV					
	Hole			Electron		
	HTC-a	HTC-b	HTC-c	HTC-a	HTC-b	HTC-c
0	0.306	0.261	0.267	0.30	0.282	0.280
10	0.226	0.194	0.20	0.185	0.181	0.175
20	0.073	0.049	0.056	0.003	0.0002	0.009
30	0.091	0.122	0.109	0.129	0.133	0.148
40	0.315	0.332	0.325	0.209	0.193	0.236
50	0.485	0.477	0.481	0.085	0.263	0.10
60	0.325	0.324	0.322	0.277	0.378	0.317
70	0.017	0.030	0.018	0.413	0.434	0.416
80	0.196	0.193	0.198	0.225	0.228	0.208
90	0.169	0.173	0.171	0.001	0.013	0.011

Table S2. The number of forward (N_f) and backward (N_b) oscillations and their probabilities (P_f and P_b), effective displacement (d_{eff}) and average site energy difference $\langle \Delta\varepsilon_{ij} \rangle$ for forward and backward motions calculated from kinetic Monte Carlo simulations

Molecules	Hole							Electron						
	N_f	N_b	P_f	P_b	d_{eff} in Å	$\langle \Delta\varepsilon_{ij} \rangle$ in eV		N_f	N_b	P_f	P_b	d_{eff} in Å	$\langle \Delta\varepsilon_{ij} \rangle$ in eV	
						Forward	Backward						Forward	Backward
HTC-a	0.98	0.85	0.54	0.46	0.27	-0.005	0.005	1	0.73	0.57	0.43	0.47	-0.007	0.007
HTC-b	1.14	0.84	0.58	0.42	0.54	-0.014	0.014	1.37	0.87	0.61	0.39	0.74	-0.02	0.02
HTC-c	2.36	0.72	0.76	0.23	1.79	-0.054	0.054	4.91	0.47	0.91	0.09	2.76	-0.13	0.13