Supplementary Materials

Fig. S1 The optimized geometry of Au and S substituted TTF based molecular wire for the various applied EFs.

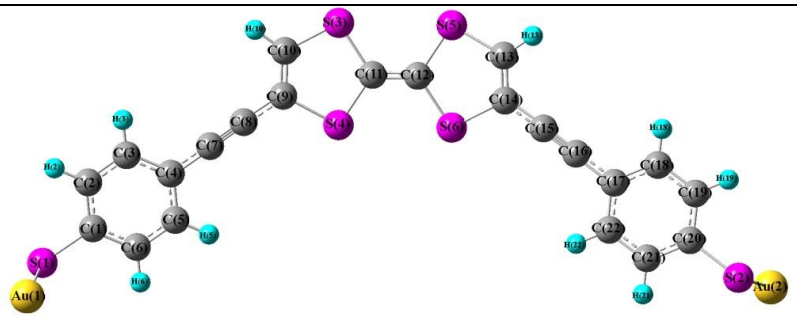
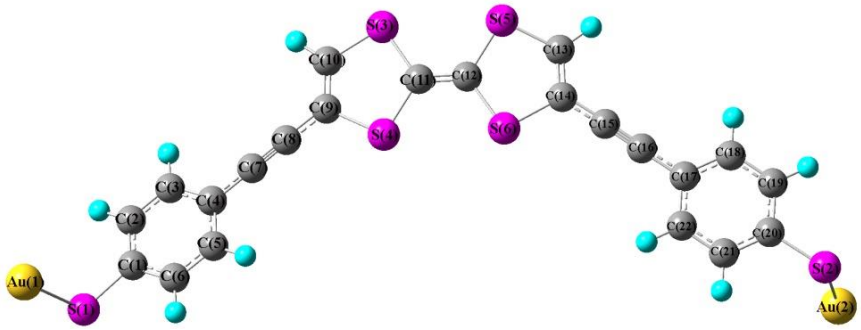
EF ($VÅ^{-1}$)	Optimized geometry
0.08	
0.16	

Fig. S2 Deformation density maps of Au and S substituted TTF based molecule for the various applied EFs. Solid lines represent positive contours, dotted lines are negative contours and dashed lines are zero contours. The contours are drawn at 0.05 $eÅ^{-3}$ intervals.

EF ($VÅ^{-1}$)	Deformation density

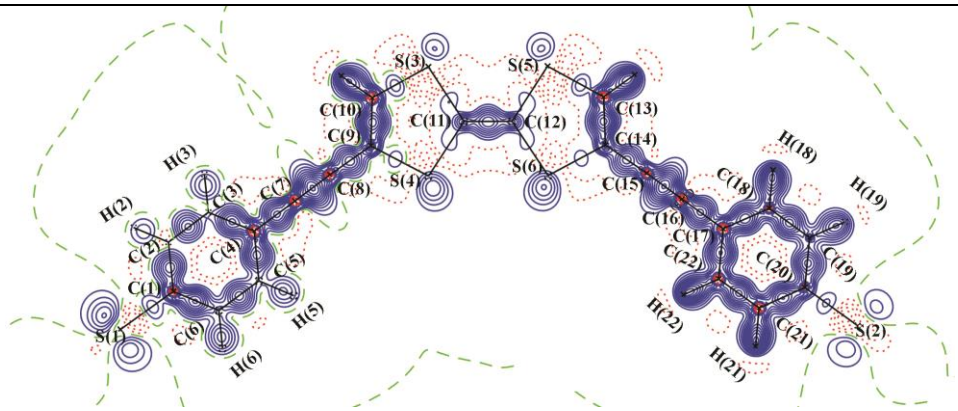
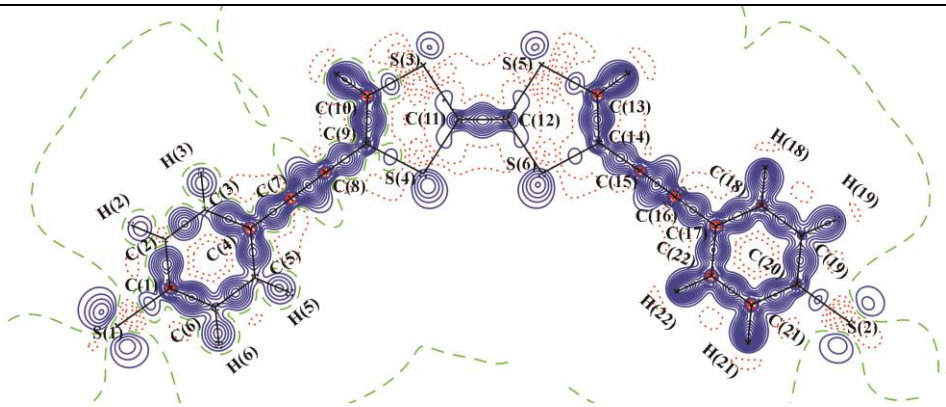
0.08	
0.16	

Fig. S3 Laplacian of electron density maps of Au and S substituted TTF based molecule for the various applied EFs. The contours are drawn in logarithmic scale, $3x2^{N}$ eÅ^{-5}, where N = 2, 4 and $8x10^{n}$, n= -2, -1, 0, 1, 2. Solid lines are positive contours and dotted lines are negative contours.

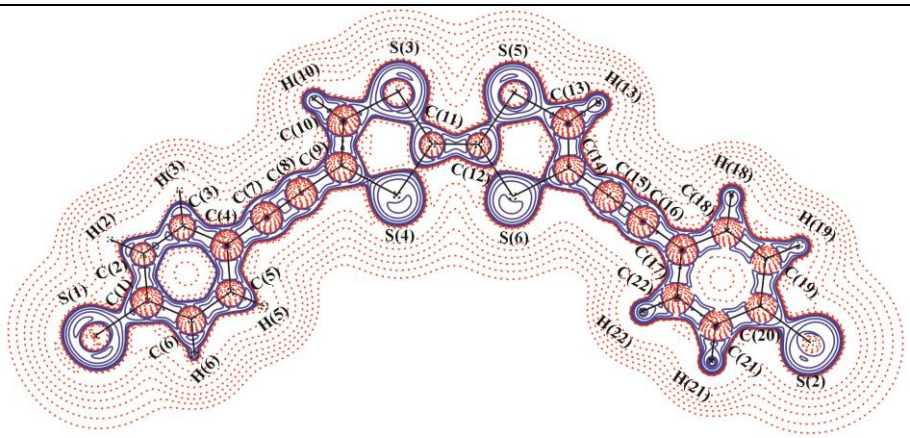
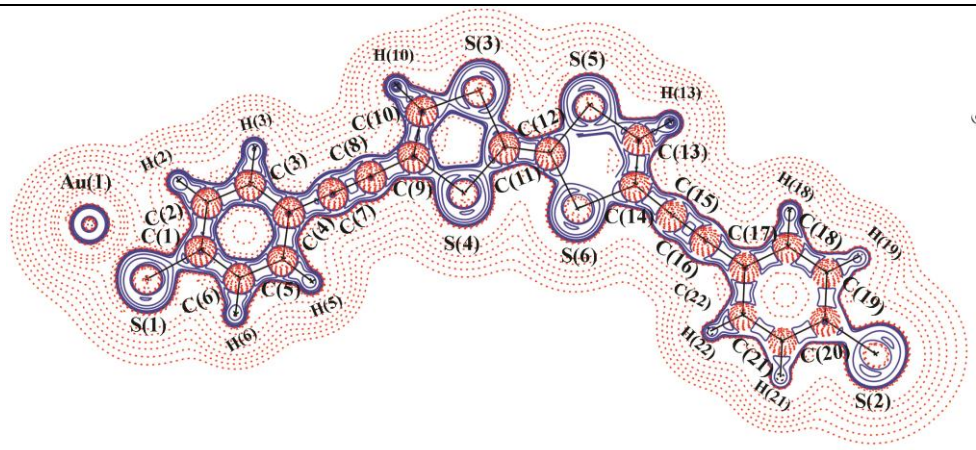
EF ($VÅ^{-1}$)	Deformation density
0.08	
0.16	

Table S1 Bond lengths (Å) of Au and S substituted TTF based molecule for the zero and various applied EFs ($VÅ^{-1}$).

Bonds	Applied electric field					
	0.00	0.04	0.08	0.12	0.16	0.20
Ring 1						
C(1)–C(2)	1.413	1.413	1.413	1.413	1.414	1.416
C(3)–C(4)	1.421	1.420	1.421	1.421	1.422	1.423
C(5–C(6)	1.401	1.401	1.401	1.400	1.400	1.396
C(1)–C(6)	1.413	1.413	1.413	1.413	1.418	1.422
Ring 2						
S(3)–C(10)	1.802	1.804	1.805	1.807	1.809	1.810
S(3) –C(11)	1.847	1.845	1.844	1.842	1.840	1.838
S(4)–C(9)	1.854	1.855	1.856	1.858	1.859	1.860
S(4)–C(11)	1.839	1.838	1.836	1.834	1.832	1.831
Ring 3						
S(5)–C(12)	1.847	1.848	1.849	1.849	1.850	1.851
S(5)–C(13)	1.802	1.800	1.796	1.796	1.793	1.789
S(6)–C(12)	1.840	1.841	1.844	1.844	1.844	1.845
S(6)–C(14)	1.854	1.853	1.852	1.852	1.851	1.851
Ring 4						
C(17)–C(18)	1.421	1.421	1.422	1.422	1.423	1.424
C(19)–C(20)	1.413	1.413	1.414	1.414	1.415	1.416
C(21)–C(22)	1.401	1.401	1.400	1.400	1.400	1.390
C(17)–C(22)	1.421	1.421	1.422	1.422	1.422	1.422

Ring Connectors						
C(4)–C(7)	1.429	1.429	1.429	1.429	1.429	1.424
C(8)–C(9)	1.411	1.411	1.411	1.411	1.409	1.406
C(11)–C(12)	1.349	1.349	1.349	1.350	1.352	1.354
C(16)–C(17)	1.429	1.428	1.427	1.427	1.427	1.427
C≡C Bonds						
C(7)–C(8)	1.229	1.229	1.229	1.229	1.230	1.232
C(15)–C(16)	1.229	1.229	1.230	1.230	1.231	1.231
C–H Bonds						
C(2)–H(2)	1.086	1.086	1.086	1.086	1.806	1.086
C(22)–H(22)	1.086	1.086	1.086	1.086	1.086	1.087
Terminal Bonds						
S(1)–C(1)	1.838	1.839	1.84	1.841	1.842	1.842
S(2)–C(20)	1.837	1.835	1.833	1.833	1.830	1.828
Au(1)–S(1)	2.401	2.399	2.396	2.395	2.392	2.388
Au(2)–S(2)	2.401	2.403	2.407	2.410	2.433	2.463

Table S2 Electron density $\rho_{bcp}(r)$ ($eÅ^{-3}$) values of Au and S substituted TTF based molecule for the zero and various applied EFs ($VÅ^{-1}$).

Bonds	Applied electric field					
	0.00	0.04	0.08	0.12	0.16	0.20
Ring 1						
C(1)–C(2)	1.912	1.913	1.913	1.913	1.913	1.893
C(3)–C(4)	1.885	1.885	1.884	1.883	1.879	1.874
C(5)–C(6)	1.949	1.949	1.946	1.945	1.945	1.964
C(1)–C(6)	1.911	1.912	1.914	1.914	1.914	1.874
Ring 2						
S(3)–C(10)	1.084	1.081	1.079	1.077	1.077	1.090
S(3)–C(11)	0.996	0.997	0.998	1.001	1.006	1.009
S(4)–C(11)	1.006	1.009	1.010	1.013	1.015	1.018
C(10)–C(9)	2.069	2.071	2.071	2.072	2.072	2.057
Ring 3						
S(5)–C(12)	0.996	0.995	0.993	0.995	0.995	0.999
S(5)–C(13)	1.084	1.088	1.095	1.094	1.099	1.108
S(6)–C(12)	1.006	1.003	0.999	1.001	0.999	0.997
C(13)–C(14)	2.069	2.067	2.063	2.062	2.059	2.054
Ring 4						
C(17)–C(18)	1.884	1.883	1.881	1.880	1.878	1.872
C(19)–C(20)	1.912	1.910	1.908	1.908	1.905	1.901
C(21)–C(22)	1.948	1.949	1.950	1.951	1.951	1.946
C(17)–C(22)	1.884	1.883	1.882	1.880	1.880	1.880

Ring Connectors						
C(4)–C(7)	1.800	1.797	1.794	1.793	1.793	1.811
C(8)–C(9)	1.850	1.851	1.852	1.853	1.861	1.869
C(11)–C(12)	2.092	2.092	2.091	2.089	2.084	2.073
C(16)–C(17)	1.800	1.804	1.809	1.810	1.810	1.809
C≡C Bonds						
C(7)–C(8)	2.477	2.478	2.477	2.477	2.477	2.467
C(15)–C(16)	2.477	2.477	2.476	2.474	2.471	2.468
C–H Bonds						
C(2)–H(2)	1.801	1.803	1.804	1.804	1.804	1.798
C(22)–H(22)	1.797	1.799	1.799	1.800	1.800	1.797
Terminal Bonds						
S(1)–C(1)	1.017	1.015	1.013	1.01	1.01	1.009
S(2)–C(20)	1.018	1.021	1.024	1.025	1.027	1.028
Au(1)–S(1)	0.520	0.522	0.525	0.528	0.532	0.538
Au(2)–S(2)	0.520	0.517	0.514	0.511	0.489	0.465

Table S3 Laplacian of electron density $\nabla^2\rho_{bcp}(r)$ ($eÅ^{-5}$) values of Au and S substituted TTF based molecule for the zero and various applied EFs ($VÅ^{-1}$).

Bonds	Applied electric field					
	0.00	0.04	0.08	0.12	0.16	0.20
Ring 1						
C(1)–C(2)	-17.624	-17.644	-17.645	-17.649	-17.649	-17.296
C(3)–C(4)	-17.264	-17.270	-17.235	-17.224	-17.165	-17.077
C(5)–C(6)	-18.465	-18.456	-18.404	-18.387	-18.380	-18.710
C(1)–C(6)	-17.616	-17.632	-17.659	-17.659	17.601	-16.931
Ring 2						
S(3)–C(10)	-5.278	-5.211	-5.175	-5.121	-5.121	-5.303
S(3)–C(11)	-3.806	-3.838	-3.862	-3.906	-3.956	-4.003
S(4)–C(9)	-3.781	-3.743	-3.722	-3.659	-3.601	-3.583
S(4)–C(11)	-3.996	-4.041	-4.074	-4.127	-4.188	-4.219
C(10)–C(9)	-19.77	-19.782	-19.785	-19.787	-19.79	-19.553
Ring 3						
S(5)–C(12)	-3.807	-3.777	-3.746	-3.758	-3.755	-3.803
S(5)–C(13)	-5.279	-5.366	-5.520	-5.513	-5.520	-5.770
S(6)–C(14)	-3.779	-3.815	-3.889	-3.844	-3.845	-3.870
C(13)–C(14)	-19.770	-19.745	-19.699	-19.676	-19.612	-19.560
Ring 4						
C(17)–C(18)	-17.255	-17.236	-17.197	-17.192	-17.124	-17.041
C(18)–C(19)	-18.436	-18.458	-18.492	-18.484	-18.499	-18.538
C(21)–C(22)	-18.454	-18.466	-18.480	-18.497	-18.434	-18.396

C(17)–C(22)	-17.247	-17.236	-17.218	-17.198	-17.190	-17.187
Ring Connectors						
C(4)–C(7)	-16.311	-16.244	-16.167	-16.135	-16.178	-16.326
C(8)–C(9)	-17.137	-17.158	-17.177	-17.196	-17.309	-17.451
C(11)–C(12)	-19.940	-19.934	-19.909	-19.888	-19.758	-19.638
C(7) ≡C(8)	-24.511	-24.506	-24.480	-24.480	-24.440	-24.382
C(15) ≡C(16)	-24.510	-24.507	-24.513	-24.492	-24.435	-24.399
C–H Bonds						
C(10)–H(10)	-21.183	-21.224	-21.272	-21.291	-21.324	-21.497
C(18)–H(18)	-20.680	-20.657	-20.633	-20.615	-20.567	-20.446
Terminal Bonds						
S(1)–C(1)	-4.207	-4.186	-4.167	-4.142	-4.123	-4.101
S(2)–C(20)	-4.217	-4.253	-4.297	-4.301	-4.345	-4.387
Au(1)–S(1)	2.950	2.971	3.014	3.024	3.218	3.409
Au(2)–S(2)	2.954	2.947	2.925	2.925	2.925	2.925

Table S4 Bond energy density ($HÅ^{-3}$) values of Au and S substituted TTF based molecule for the zero and various applied EFs ($VÅ^{-1}$).

Bonds	Applied electric field					
	0.00	0.04	0.08	0.12	0.16	0.20
Ring 1						
C(1)–C(2)	-1.864	-1.864	-1.864	-1.864	-1.865	-1.837
C(3)–C(4)	-1.815	-1.816	-1.814	-1.813	-1.792	-1.795
C(5)–C(6)	-1.944	-1.944	-1.938	-1.936	-1.936	-1.977
C(1)–C(6)	-1.862	-1.863	-1.866	-1.866	-1.866	-1.797
Ring 2						
S(3)–C(10)	-0.710	-0.702	-0.697	-0.691	-0.686	-0.707
S(3)–C(11)	-0.587	-0.592	-0.596	-0.602	-0.608	-0.614
S(4)–C(9)	-0.572	-0.568	-0.565	-0.560	-0.557	-0.552
S(4)–C(11)	-0.609	-0.616	-0.621	-0.627	-0.638	-0.640
C(10)–C(9)	-2.212	-2.217	-2.219	-2.220	-2.220	-2.187
Ring 3						
S(5)–C(12)	-0.587	-0.583	-0.578	-0.579	-0.580	-0.584
S(5)–C(13)	-0.710	-0.720	-0.737	-0.738	-0.744	-0.763
S(6)–C(12)	-0.609	-0.603	-0.595	-0.597	-0.593	-0.591
S(6)–C(14)	-0.572	-0.577	-0.584	-0.581	-0.581	-0.583
C(13)–C(14)	-2.212	-2.207	-2.199	-2.195	-2.189	-2.178
Ring 4						
C(17)–C(18)	-1.814	-1.811	-1.806	-1.805	-1.796	-1.789
C(18)–C(19)	-1.941	-1.944	-1.948	-1.948	-1.952	-1.956

C(21)–C(22)	-1.943	-1.944	-1.946	-1.948	-1.948	-1.940
C(17)–C(22)	-1.813	-1.811	-1.808	-1.806	-1.805	-1.805
Ring Connectors						
C(4)–C(7)	-1.705	-1.704	-1.703	-1.703	-1.703	-1.748
C(8)–C(9)	-1.783	-1.782	-1.782	-1.784	-1.784	-1.816
C(11)–C(12)	-2.268	-2.266	-2.264	-2.259	-2.252	-2.226
C(16)–C(17)	-1.706	-1.709	-1.716	-1.719	-1.821	-1.718
C(7) ≡C(8)	-3.241	-3.241	-3.240	-3.241	-3.241	-3.217
C(15) ≡C(16)	-3.241	-3.239	-3.238	-3.235	-3.227	-3.219
C–H Bonds						
C(18)–H(18)	-1.733	-1.732	-1.730	-1.730	-1.726	-1.722
C(10)–H(10)	-1.759	-1.760	-1.762	-1.763	-1.767	-1.772
Terminal Bonds						
S(1)–C(1)	-0.619	-0.618	-0.617	-0.615	-0.616	-0.671
S(2)–C(20)	-0.621	-0.624	-0.628	-0.629	-6.400	-0.646
Au(1)–S(1)	-0.156	-0.157	-0.159	-0.157	-0.146	-0.161
Au(2)–S(2)	-0.156	-0.155	-0.153	-0.151	-0.144	-0.124

Table S5 Atomic charges (e) of Au and S substituted TTF based molecule for the zero and various applied EFs (first line CHELPG charges, second line MK charges).

Atom	Applied electric field ($VÅ^{-1}$)					
	0.00	0.04	0.08	0.12	0.16	0.20
C(1)	0.291	0.273	0.278	0.275	0.275	0.262
	0.174	0.177	0.172	0.172	0.167	0.167
C(4)	0.181	0.175	0.157	0.200	0.200	0.194

	0.179	0.169	0.161	0.197	0.197	0.144
C(7)	-0.125	-0.132	-0.116	-0.152	-0.152	-0.153
	-0.072	-0.061	-0.055	-0.109	-0.109	-0.021
C(9)	0.132	0.104	0.113	0.104	0.104	0.098
	0.153	0.164	0.168	0.143	0.143	0.181
C(10)	-0.182	-0.150	-0.157	-0.174	-0.174	-0.148
	-0.265	-0.268	-0.266	-0.269	-0.269	-0.277
C(12)	0.053	0.034	0.024	0.030	0.030	0.039
	-0.028	-0.023	-0.028	-0.027	-0.027	-0.042
C(13)	-0.165	-0.189	-0.182	-0.179	-0.179	-0.176
	-0.292	-0.289	-0.288	-0.291	-0.291	-0.297
C(14)	0.106	0.132	0.117	0.132	0.132	0.114
	0.176	0.170	0.171	0.181	0.181	0.206
C(15)	-0.029	-0.053	-0.038	-0.060	-0.060	-0.048
	-0.118	-0.112	-0.115	-0.131	-0.131	-0.145
C(17)	0.167	0.146	0.154	0.154	0.154	0.151
	0.202	0.198	0.203	0.240	0.240	0.237
C(20)	0.306	0.288	0.289	0.287	0.287	0.322
	0.168	0.175	0.177	0.099	0.099	0.193
S(3)	-0.034	-0.044	-0.040	-0.037	-0.037	-0.041
	0.002	0.006	0.006	0.005	0.005	-0.002
S(6)	-0.069	-0.071	-0.065	-0.068	-0.068	-0.068
	-0.039	-0.039	-0.036	-0.040	-0.040	-0.046
H(2)	0.069	0.069	0.073	0.076	0.076	0.058
	0.103	0.103	0.099	0.111	0.111	0.080

H(22)	0.155	0.150	0.151	0.155	0.155	0.149
	0.201	0.199	0.198	0.207	0.207	0.205
S(1)	-0.333	-0.332	-0.332	-0.331	-0.331	-0.331
	-0.302	-0.303	-0.302	-0.307	-0.307	-0.293
S(2)	-0.333	-0.333	-0.333	-0.333	-0.333	-0.348
	-0.303	-0.303	-0.303	-0.307	-0.307	-0.310
Au(1)	0.175	0.177	0.177	0.179	0.181	0.183
	0.156	0.157	0.157	0.159	0.161	0.165
Au(2)	0.177	0.177	0.177	0.176	0.176	0.176
	0.159	0.158	0.158	0.158	0.156	0.155