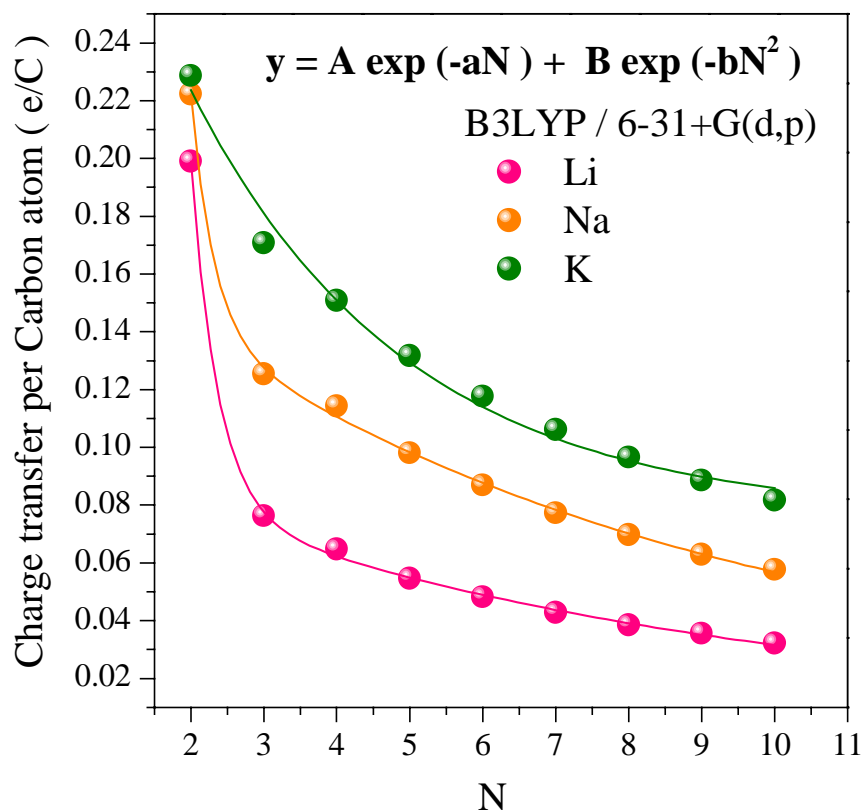


# **SUPPORTING INFORMATION FILE**

**Manuscript Number: jp0731147**

**Role of charge transfer interaction and conjugation length on electrical polarizability of doped trans-polyacetylene oligomer**

**Sabyasachi Sen and Swapan Chakrabarti**



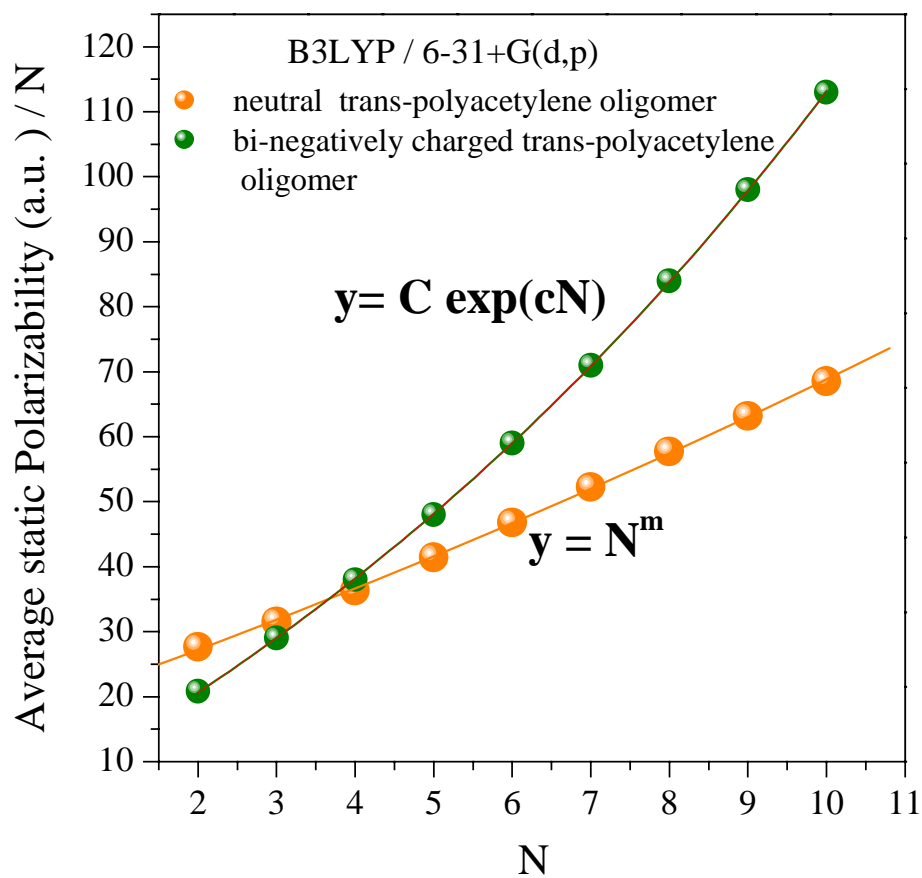
**Figure F1:** Second order exponential fit for the variation of charge transfer per carbon atom (e/C) from metal atoms to trans-polyacetylene back bone (B3LYP/6-31+G(d, p) results).

**Second order exponential fit:**

CHI SQUARE FIT :  $5.0005 \times 10^{-7}$  FOR Li DOPING  
 $5.0012 \times 10^{-6}$  FOR Na DOPING  
 $1.1644 \times 10^{-6}$  FOR K DOPING

**First order exponential fit:**

CHI SQUARE FIT :  $8.0 \times 10^{-5}$  FOR Li DOPING  
 $13.0 \times 10^{-5}$  FOR Na DOPING  
 $3.0 \times 10^{-5}$  FOR K DOPING



**Figure F2:** First order exponential fit for neutral and bi-negatively charged trans-polyacetylene oligomer

CHI SQUARE FIT for bi-negatively charged trans-polyacetylene oligomer : 0.03649

CHI SQUARE FIT for pristine trans-polyacetylene oligomer : 0.12

TABLE I : POWER LAW EXPONENTS AND CHOSEN COEFFICIENTS FOR ALL THE DOPANTS

Sample	Mathematical form: [ $A_1 \exp(-aN) + B_1 \exp(-bN^2) + C_1 \exp(cN)$ ]	
	Values of exponents	Chosen coefficients
Li doped trans-polyacetylene oligomer	a= 2.807, b=0.203, c=0.060,	$A_1=3, B_1=136, C_1=116$
Na doped trans-polyacetylene oligomer	a= 2.807, b=0.143, c=0.050,	$A_1=3, B_1=185, C_1=167$
K doped trans-polyacetylene oligomer	a= 2.807, b=0.143, c=0.027,	$A_1=3, B_1=272, C_1=257$

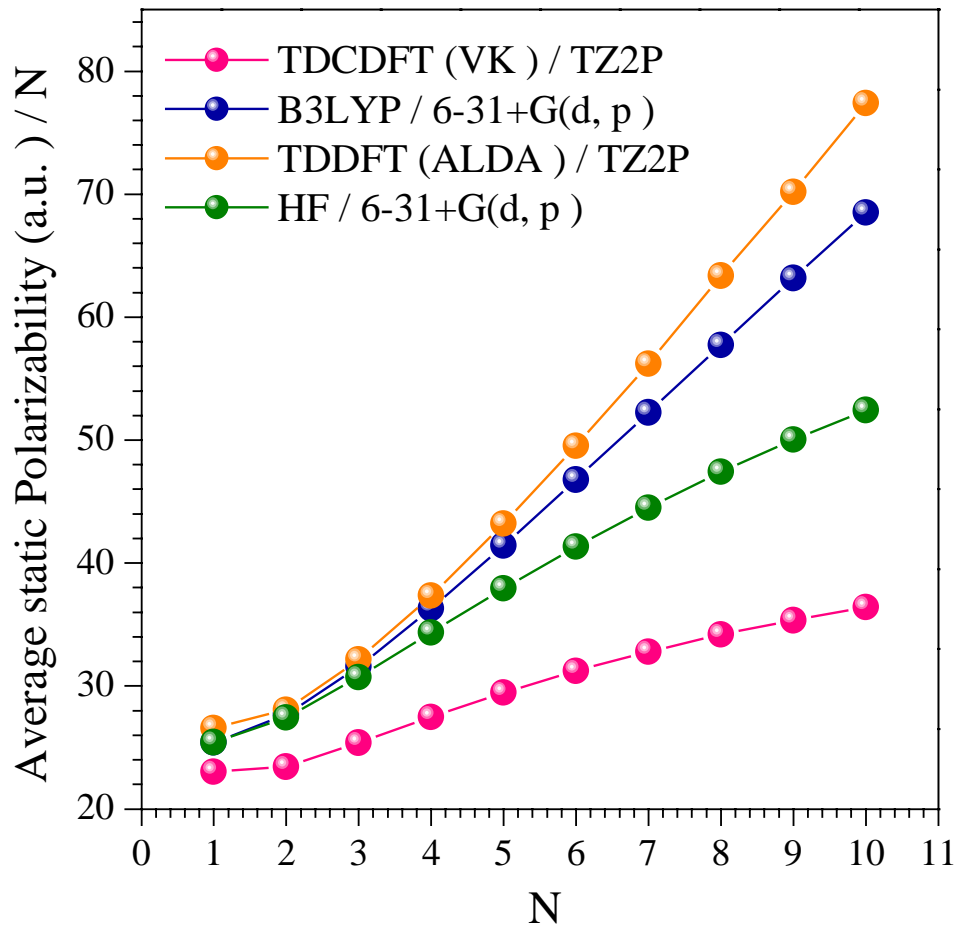
## Different components of static polarizability in case of undoped trans-polyacetylene oligomer

N	Transverse polarizability ( $\alpha_{zz}$ ) (B3LYP)	Transverse polarizability ( $\alpha_{yy}$ ) (B3LYP)	Average Transverse polarizability ( $(\alpha_{zz} + \alpha_{yy})/2$ ) (B3LYP)	Axial polarizability ( $\alpha_{xx}$ ) (B3LYP)
1	22.5294	18.4172	20.4733	35.2849
2	23.0015	16.4257	19.7136	43.5391
3	25.0506	15.2088	20.1297	54.4554
4	27.7479	14.5628	21.1553	66.5646
5	30.7757	14.1579	22.4668	79.3364
6	33.9959	13.8814	23.9386	92.4696
7	37.3100	13.6781	25.4940	105.7408
8	40.6733	13.5264	27.0998	118.9858
9	44.0259	13.4077	28.7168	132.0698
10	47.3277	13.3101	30.3189	144.8882

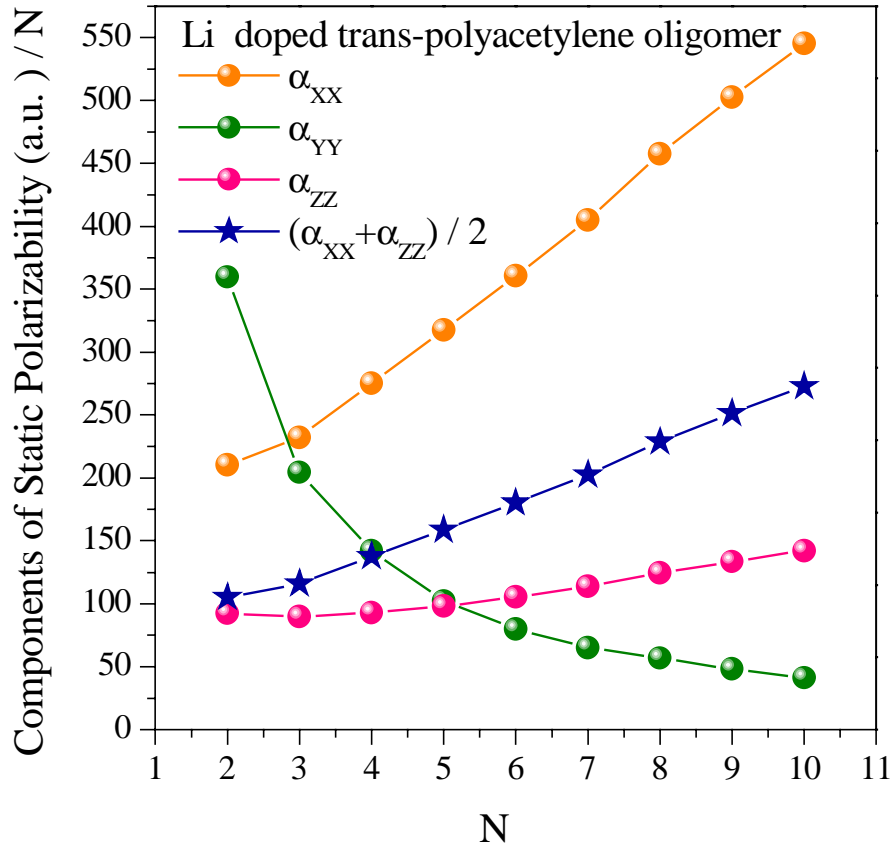
N	Transverse polarizability ( $\alpha_{zz}$ ) (HF)	Transverse polarizability ( $\alpha_{yy}$ ) (HF)	Average Transverse polarizability ( $(\alpha_{zz} + \alpha_{yy})/2$ ) (HF)	Axial polarizability ( $\alpha_{xx}$ ) (HF)
1	21.7973	18.0567	19.9270	36.4280
2	21.1210	16.2593	18.6901	44.9080
3	22.1509	15.1002	18.6255	54.9118
4	23.5763	14.4750	19.0256	64.9672
5	25.0905	14.0844	19.5874	74.6079
6	26.5793	13.8179	20.1986	83.6223
7	27.9824	13.6220	20.8022	91.9155
8	29.2880	13.4759	21.3819	99.4732
9	30.4817	13.3615	21.9216	106.3159
10	31.5631	13.2677	22.4154	112.4886

N	Transverse polarizability ( $\alpha_{ZZ}$ ) (TDCDFT)	Transverse polarizability ( $\alpha_{YY}$ ) (TDCDFT)	Average Transverse polarizability ( $(\alpha_{ZZ} + \alpha_{YY})/2$ ) (TDCDFT)	Axial polarizability ( $\alpha_{XX}$ ) (TDCDFT)
1	22.4064	14.5498	18.4781	32.1551
2	21.8337	12.6620	17.2478	35.8125
3	22.8490	11.9527	17.4008	41.3624
4	24.1755	11.5492	17.8623	46.7363
5	25.4990	11.2986	18.3988	51.5775
6	26.7217	11.1289	18.9253	55.8381
7	27.8209	11.0063	19.4136	59.5559
8	28.8242	10.9163	19.8702	62.7965
9	29.6297	10.8360	20.2328	65.5543
10	30.3958	10.7838	20.5898	68.067

N	Transverse polarizability ( $\alpha_{ZZ}$ ) (ALDA)	Transverse polarizability ( $\alpha_{YY}$ ) (ALDA)	Average Transverse polarizability ( $(\alpha_{ZZ} + \alpha_{YY})/2$ ) (ALDA)	Axial polarizability ( $\alpha_{XX}$ ) (ALDA)
1	25.1316	18.7173	21.9244	35.9202
2	24.7512	16.1785	20.4648	43.2702
3	26.8452	15.1286	20.9869	54.5136
4	29.9107	14.5394	22.2250	67.5879
5	33.5363	14.1709	23.8536	81.8819
6	37.5386	13.9217	25.7301	97.0935
7	41.8166	13.7417	27.7791	113.0179
8	46.4284	13.6013	30.0148	130.0813
9	50.8479	13.4993	32.1736	146.2205
10	55.6020	13.4211	34.5115	163.1647

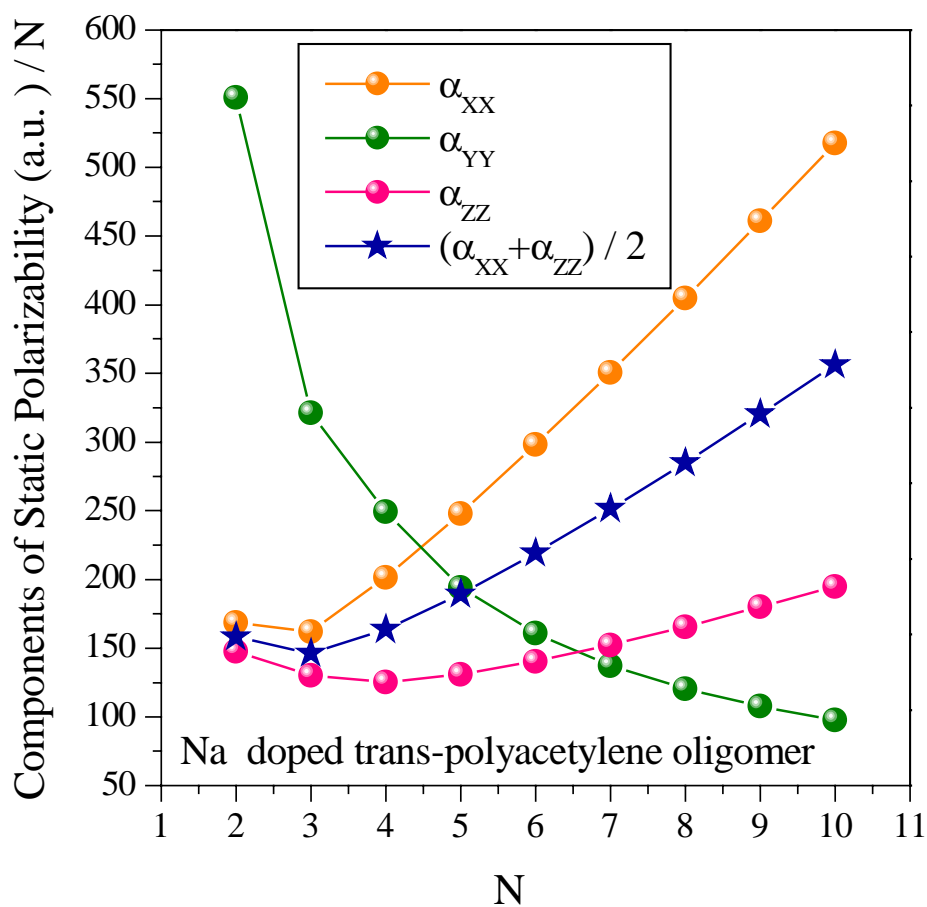


**Figure F3:** Variation of average static polarizability per acetylene unit against  $N$  for undoped trans-polyacetylene oligomer.

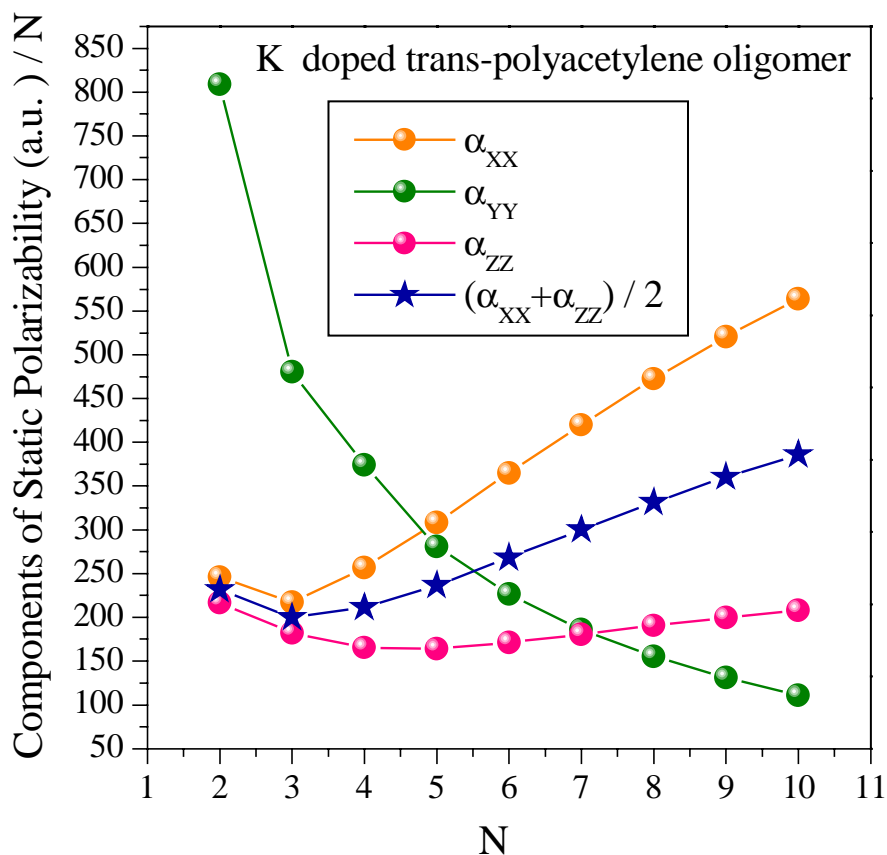


**Figure F4:** Variation of different components of static polarizability ( $\alpha_{xx}$ ,  $\alpha_{yy}$ ,  $\alpha_{zz}$ ) and average of static polarizability components not related to charge transfer interaction  $[(\alpha_{xx} + \alpha_{zz})/2]$  per acetylene unit is plotted against  $N$  for Li doped trans-polyacetylene oligomer estimated at DFT/B3LYP level of theory.





**Figure F5:** Variation of different components of static polarizability ( $\alpha_{XX}$ ,  $\alpha_{YY}$ ,  $\alpha_{ZZ}$ ) and average of static polarizability components not related to charge transfer interaction  $[(\alpha_{XX} + \alpha_{ZZ})/2]$  per acetylene unit is plotted against  $N$  for Na doped trans-polyacetylene oligomer estimated at DFT/B3LYP level of theory.



**Figure F6:** Variation of different components of static polarizability ( $\alpha_{XX}$ ,  $\alpha_{YY}$ ,  $\alpha_{ZZ}$ ) and average of static polarizability components not related to charge transfer interaction [ $(\alpha_{XX} + \alpha_{ZZ}) / 2$ ] per acetylene unit is plotted against  $N$  for K doped trans-polyacetylene oligomer estimated at DFT/B3LYP level of theory.