Supporting Information:

Polaron Localization in π-Conjugated Polymers Cations by Long Range Corrected DFT Methods

Nan Shao[a] and Qin Wu[a]

[a] *Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973, USA*

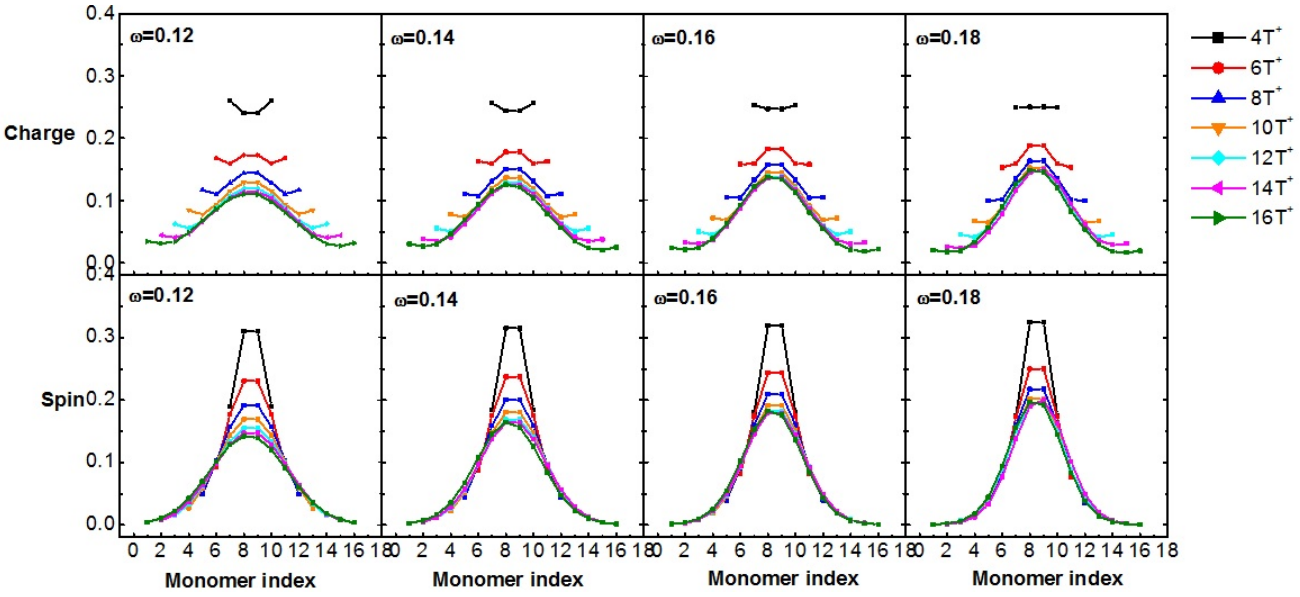
Email Address: qinwu@bnl.gov

SF1. Charge and spin distribution of nT+ with length from 4 to 16 for range parameter ω=0.12, 0.14, 0.16 and 0.18 $bohr^{-1}$.

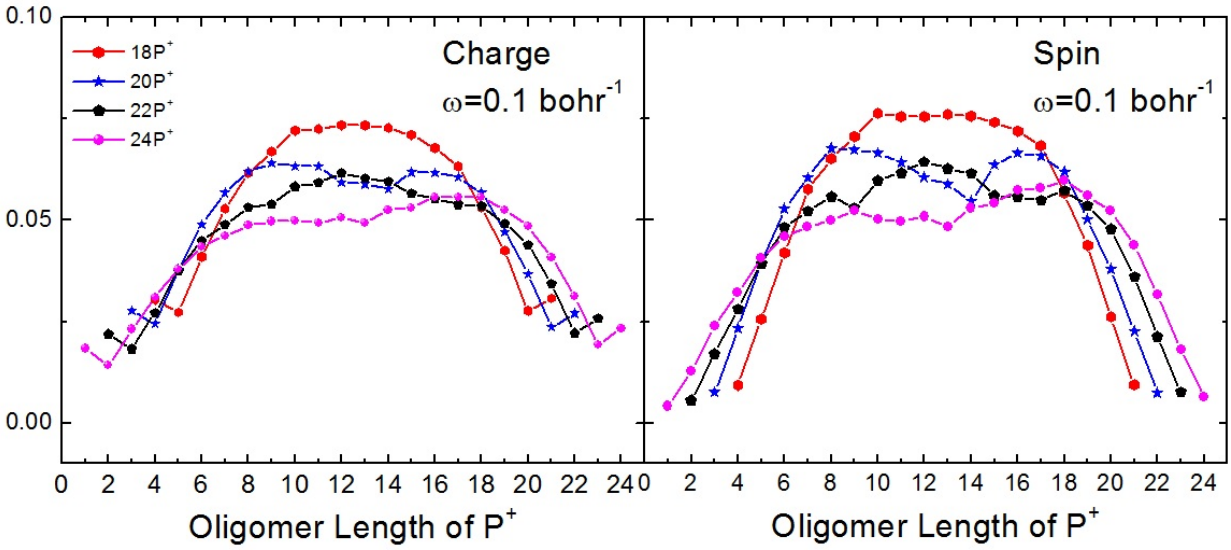
SF2. Charge and spin distribution of nP+ with length from 18 to 24 for ω=0.1 $bohr^{-1}$.

ST1. Reorganization energies of five polymers with ωPBE (ω =0.1~0.4 $bohr^{-1}$).

ST2. Excitation energies (first) of five polymers with ωPBE (ω =0.1~0.4 $bohr^{-1}$).



SF1. Charge and spin distribution of nT+ with length from 4 to 16 for range parameter ω=0.12, 0.14, 0.16 and 0.18 bohr^{-1}.



SF2. Charge and spin distribution of nP+ with length from 18 to 24 for ω=0.1 bohr^{-1}.

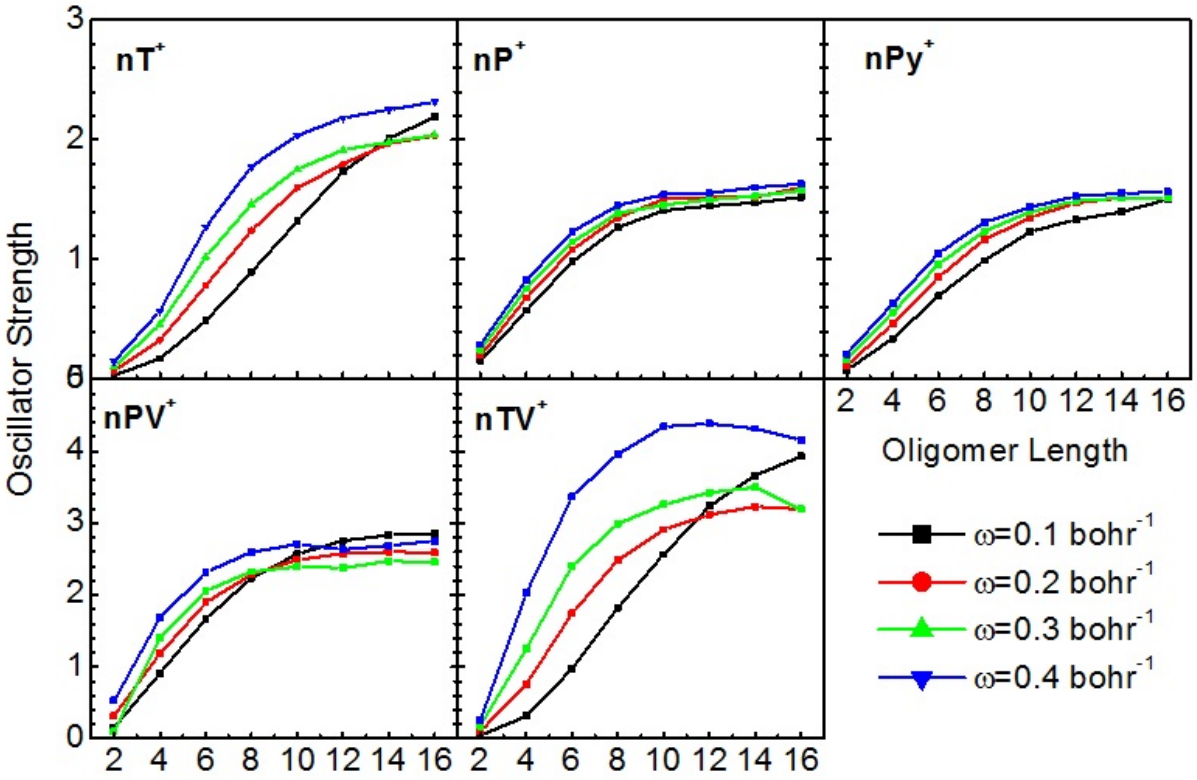
ST 1. Reorganization energies (eV)

Polymer	ω (bohr^{-1})	n=2	4	6	8	10	12	14	16
nT	**0.1**	0.31	0.26	0.27	0.23	0.21	0.23	0.21	0.21
	0.2	0.40	0.53	0.54	0.60	0.53	0.53	0.52	0.52
	0.3	0.62	0.69	0.77	0.79	0.74	0.74	0.72	0.73
	0.4	0.70	0.81	0.88	0.95	0.90	0.90	0.88	0.87
nP	**0.1**	0.31	0.33	0.28	0.24	0.18	0.17	0.14	0.11
	0.2	0.41	0.46	0.43	0.41	0.39	0.38	0.40	0.38
	0.3	0.50	0.58	0.54	0.55	0.55	0.55	0.55	0.54
	0.4	0.57	0.65	0.64	0.64	0.64	0.64	0.67	0.64
nPy	**0.1**	0.40	0.36	0.32	0.29	0.26	0.20	0.18	0.16
	0.2	0.52	0.54	0.55	0.53	0.53	0.48	0.44	0.46
	0.3	0.64	0.70	0.73	0.76	0.72	0.66	0.66	0.66
	0.4	0.72	0.82	0.83	0.90	0.83	0.84	0.79	0.78
nPV	**0.1**	0.22	0.20	0.18	0.15	0.12	0.10	0.09	0.07
	0.2	0.33	0.35	0.33	0.32	0.31	0.31	0.31	0.31
	0.3	0.49	0.57	0.60	0.61	0.58	0.52	0.53	0.53
	0.4	0.60	0.71	0.73	0.74	0.73	0.70	0.70	0.70
nTV	**0.1**	0.27	0.26	0.27	0.26	0.24	0.23	0.23	0.21
	0.2	0.40	0.47	0.51	0.51	0.51	0.50	0.50	0.53
	0.3	0.54	0.65	0.80	0.87	0.82	0.73	0.72	0.73
	0.4	0.66	0.83	1.15	1.14	1.15	1.16	1.13	1.13

ST 2. The lowest excitation energy (in eV, bold fonts) with significant strength (*italic* fonts) of the charged oligomers as calculated by TDDFT.

Polymer	ω (bohr^{-1})	n=2	4	6	8	10	12	14	16
nT	**0.1**	**2.2456**	**1.2690**	**0.8990**	**0.6820**	**0.5367**	**0.4324**	**0.3546**	**0.2888**
		0.0327	*0.1741*	*0.4878*	*0.8960*	*1.3203*	*1.7337*	*2.0076*	*2.1926*
	0.2	**2.3324**	**1.3653**	**0.9552**	**0.7184**	**0.5902**	**0.5515**	**0.5180**	**0.5139**
		0.0661	*0.3250*	*0.7822*	*1.2424*	*1.5975*	*1.7966*	*1.9700*	*2.0316*
	0.3	**2.4235**	**1.4816**	**1.0553**	**0.8618**	**0.7780**	**0.7517**	**0.7462**	**0.7383**
		0.1071	*0.4559*	*1.0215*	*1.4629*	*1.7521*	*1.9149*	*1.9816*	*2.0384*
	0.4	**2.5117**	**1.5957**	**1.1660**	**0.9680**	**0.9144**	**0.8964**	**0.8946**	**0.8891**
		0.1478	*0.5715*	*1.2727*	*1.7749*	*2.0354*	*2.1813*	*2.2517*	*2.3151*
nP	**0.1**	**2.0476**	**1.1552**	**0.7565**	**0.5312**	**0.3780**	**0.2817**	**0.2198**	**0.1805**
		0.1520	*0.5743*	*0.9804*	*1.2693*	*1.4081*	*1.4483*	*1.4749*	*1.5208*
	0.2	**2.0584**	**1.1475**	**0.7652**	**0.5943**	**0.4956**	**0.4851**	**0.4972**	**0.4711**
		0.1985	*0.6779*	*1.0825*	*1.3506*	*1.5034*	*1.5179*	*1.5181*	*1.6046*
	0.3	**2.0944**	**1.2322**	**0.8697**	**0.7580**	**0.7612**	**0.7388**	**0.7375**	**0.7233**
		0.2461	*0.7575*	*1.1447*	*1.3849*	*1.4543*	*1.5018*	*1.5280*	*1.5763*
	0.4	**2.1550**	**1.3262**	**0.9894**	**0.8978**	**0.8696**	**0.8801**	**0.8896**	**0.8845**
		0.2894	*0.8295*	*1.2304*	*1.4509*	*1.5437*	*1.5555*	*1.6017*	*1.6297*
nPy	**0.1**	**2.4944**	**1.4007**	**0.9384**	**0.6728**	**0.5057**	**0.3913**	**0.3111**	**0.2537**
		0.0766	*0.3410*	*0.6943*	*0.9901*	*1.2315*	*1.3330*	*1.3985*	*1.5018*
	0.2	**2.5156**	**1.4267**	**0.9574**	**0.7071**	**0.5916**	**0.5401**	**0.4839**	**0.5116**
		0.1159	*0.4613*	*0.8526*	*1.1657*	*1.3487*	*1.4742*	*1.5151*	*1.5129*
	0.3	**2.5530**	**1.4961**	**1.0463**	**0.8473**	**0.7749**	**0.7570**	**0.7391**	**0.7447**
		0.1700	*0.5589*	*0.9607*	*1.2355*	*1.3958*	*1.4896*	*1.5120*	*1.5102*
	0.4	**2.6156**	**1.5735**	**1.1413**	**0.9835**	**0.9259**	**0.9008**	**0.8969**	**0.8929**
		0.2107	*0.6322*	*1.0528*	*1.3084*	*1.4361*	*1.5280*	*1.5524*	*1.5638*

nPV	**0.1**	**1.5306**	**0.8853**	**0.5680**	**0.3882**	**0.2773**	**0.2066**	**0.1620**	**0.1291**
		0.1559	*0.9119*	*1.6664*	*2.2346*	*2.5677*	*2.7543*	*2.8313*	*2.8535*
	0.2	**1.6307**	**0.8878**	**0.5872**	**0.4726**	**0.4369**	**0.4287**	**0.4329**	**0.4421**
		0.3202	*1.1815*	*1.8924*	*2.2856*	*2.4891*	*2.5787*	*2.5993*	*2.5875*
	0.3	**1.5622**	**0.9754**	**0.7260**	**0.6683**	**0.6786**	**0.6833**	**0.6650**	**0.6748**
		0.1055	*1.4059*	*2.0558*	*2.3236*	*2.3897*	*2.3768*	*2.4705*	*2.4572*
	0.4	**1.8374**	**1.0791**	**0.8709**	**0.8192**	**0.8031**	**0.8354**	**0.8380**	**0.8196**
		0.5290	*1.6818*	*2.3132*	*2.5978*	*2.7055*	*2.6321*	*2.6901*	*2.7511*
nTV	**0.1**	**1.5515**	**0.9304**	**0.6737**	**0.5171**	**0.4045**	**0.3325**	**0.2860**	**0.2553**
		0.0435	*0.3157*	*0.9751*	*1.8258*	*2.5607*	*3.2336*	*3.6636*	*3.9299*
	0.2	**1.7073**	**1.0588**	**0.7680**	**0.6304**	**0.5783**	**0.5632**	**0.5586**	**0.5656**
		0.1039	*0.7598*	*1.7454*	*2.4854*	*2.9080*	*3.1159*	*3.2273*	*3.1921*
	0.3	**1.8548**	**1.1980**	**0.9069**	**0.8152**	**0.7907**	**0.7813**	**0.7812**	**0.8077**
		0.1811	*1.2532*	*2.4031*	*2.9893*	*3.2559*	*3.4263*	*3.4992*	*3.1903*
	0.4	**1.9839**	**1.3130**	**0.9958**	**0.9088**	**0.8767**	**0.8738**	**0.9015**	**0.9120**
		0.2603	*2.0235*	*3.3724*	*3.9616*	*4.3402*	*4.3838*	*4.3136*	*4.1541*



SF3. Oscillator strength of the first excitation as calculated with TDDFT for PT^+, PP^+, PPy^+, PPV^+ and PTV^+ as a function of the oligomer length.