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

Assessing long-range corrected functionals with physically-adjusted range-separated parameter for calculating the polarizability and the second hyperpolarizability of polydiacetylene and polybutatriene chains.

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SUPPORTING INFORMATION

Table S1. Longitudinal linear polarizability and second hyperpolarizability for increasingly large PDA oligomers calculated using the 6-31G(d) basis set and different levels of approximation.

N	LC-BLYP (μ adj.)	LC-BLYP (μ = 0.47)	CAMB3LYP	CCSD(T)
	α (a.u.)			
1	125.95	122.14	129.14	113.23
2	300.43	275.33	304.86	249.20
3	543.17	463.32	532.93	413.42
4	847.10	670.20	793.98	592.20
5	1175.71	887.15	1074.66	779.02
6	1544.46	1109.56	1366.91	969.96
	γ (x 10^3 a.u.)			
1	70	62	73	
2	714	536	752	537
3	3262	1933	3216	1898
4	9823	4438	8552	4240
5	21220	7904	17093	7880
6	39486	12075	28506	12300

Table S2. Longitudinal linear polarizability and second hyperpolarizability for increasingly large PBT oligomers calculated using the 6-31G(d) basis set and different levels of approximation.

N	LC-BLYP (μ adj.)	LC-BLYP (μ = 0.47)	CAMB3LYP	CCSD(T)
	α (a.u.)			
1				
2	294.79	290.06	300.62	250.62
3	644.25	604.23	649.28	504.42
4	1161.14	1022.02	1138.72	833.26
5	1845.90	1524.37	1758.43	1225.14
6	2721.15	2091.85	2491.92	
	γ (x 10^3 a.u.)			
1				
2	226	213	198	355
3	2128	1888	1985	2429
4	10136	8007	9563	9090
5	33882	22780	31154	22800
6	90730	50236	78579	

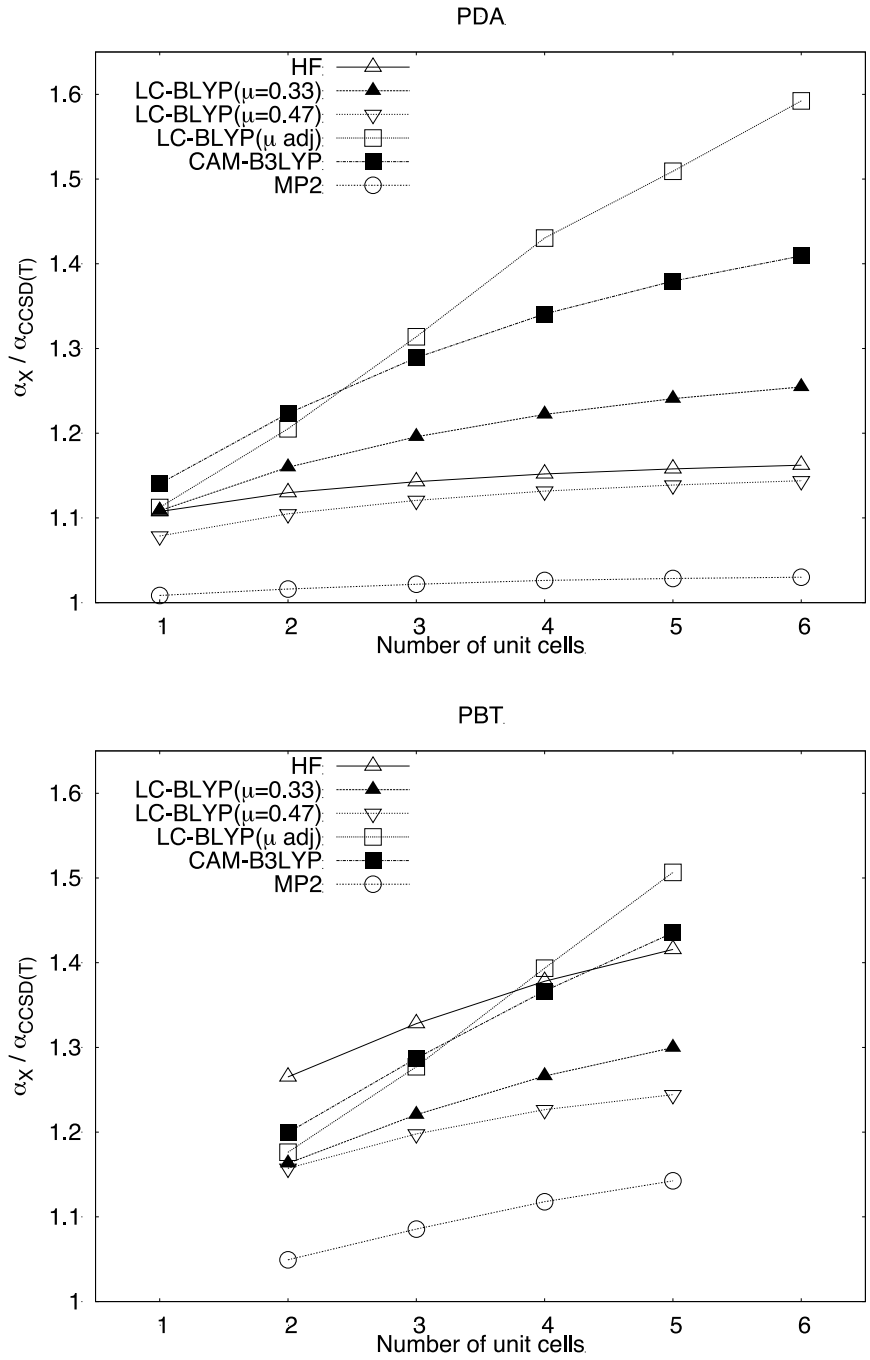

Figure S1. Evolution with chain length of the $\alpha_X/\alpha_{CCSD(T)}$ ratios for PDA (top) and PBT (bottom) chains as determined from 6-31G(d) calculations.

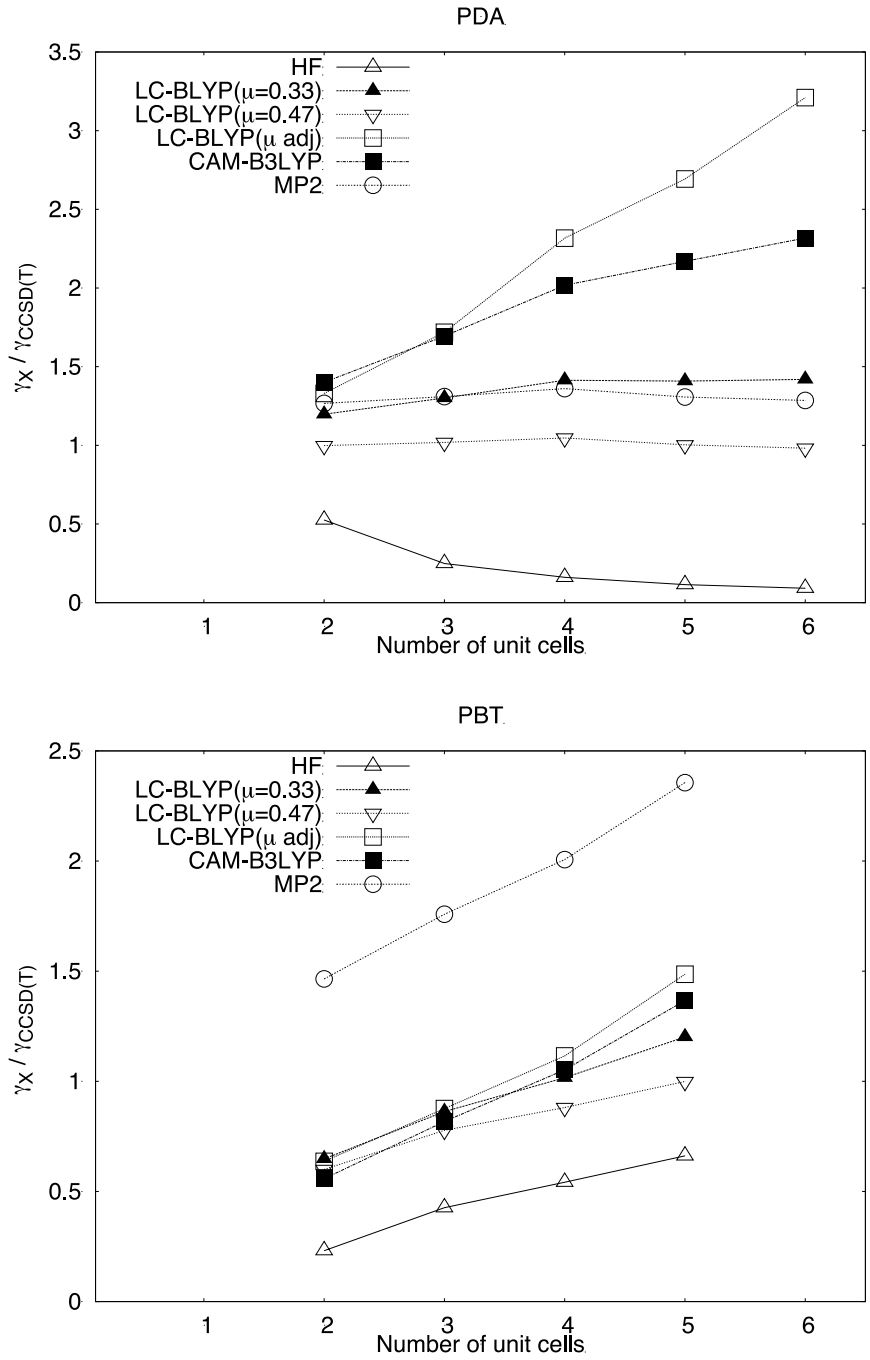

Figure S2. Evolution with chain length of the $\gamma_X/\gamma_{CCSD(T)}$ ratios for PDA (top) and PBT (bottom) chains as determined from 6-31G(d) calculations.