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Table S1 Average static first hyperpolarizability (β'_{tot}) and their corresponding x, y, and z components (β'_x, β'_y, and β'_z) of the double-helix P_nLi_n (n = 6-12) chains at LC-BLYP/6-31+G(d) theoretical level.

	β'_x (au)	β'_y (au)	β'_z (au)	β'_{tot} (au)
P_6Li_6	-1869.28	-133.03	14.25	1874.06
P_7Li_7	3514.16	669.43	232.73	3584.92
P_8Li_8	-7228.12	-1063.58	92.06	7306.53
P_9Li_9	-11768.75	392.82	920.65	11811.24
$P_{10}Li_{10}$	19145.78	-119.48	401.22	19150.36
$P_{11}Li_{11}$	-29090.80	-256.14	357.21	29094.13
$P_{12}Li_{12}$	40251.61	614.96	-724.41	40262.83

Fig S1 HOMO and LUMO distributions of the double-helix P_nLi_n (n = 6-12) chains.