Supporting Information

External Electric field Driven Electronic Structures:
Tunable Nonlinear Optical Properties in Helical Bilayer Nanographenes

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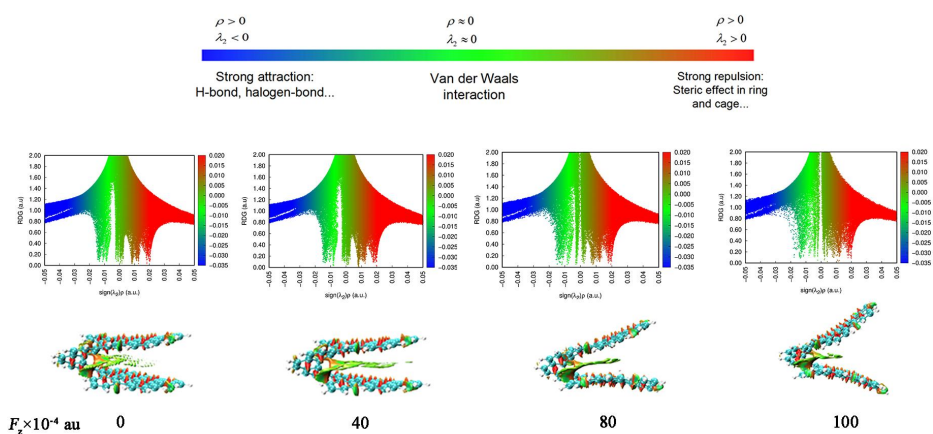E-mail: hlxu@nenu.edu.cn

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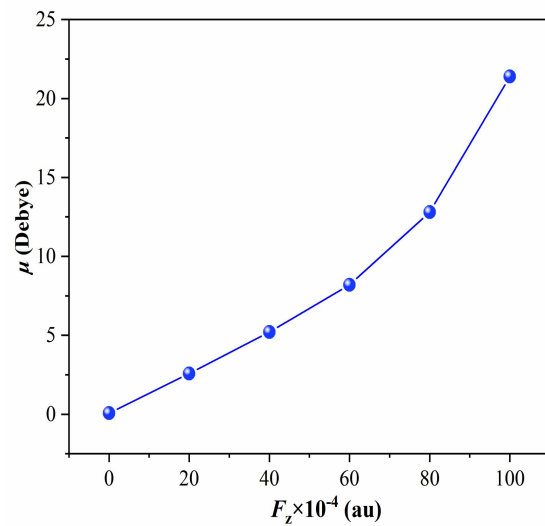
Figure S2. Evolutions of dipole moment (μ) of ground state under the vertical F_z ($F_z = 1\times10^{-4}$, au).
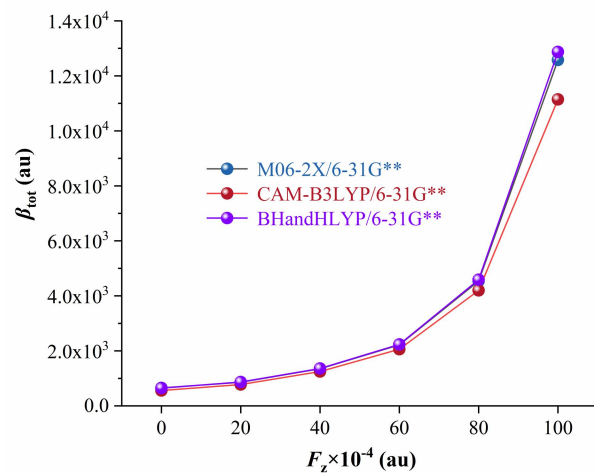
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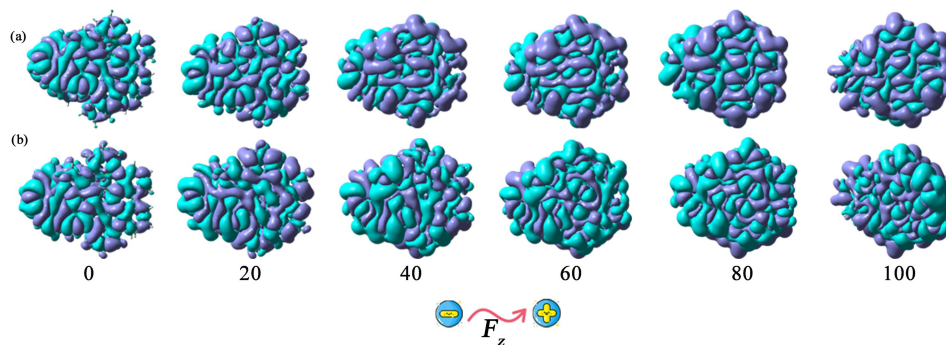
Figure S4. Evolutions of the electron density difference maps (EDDM) of the [9]HBNG under the vertical F_z ($F_z = 1\times10^{-4}$, au).
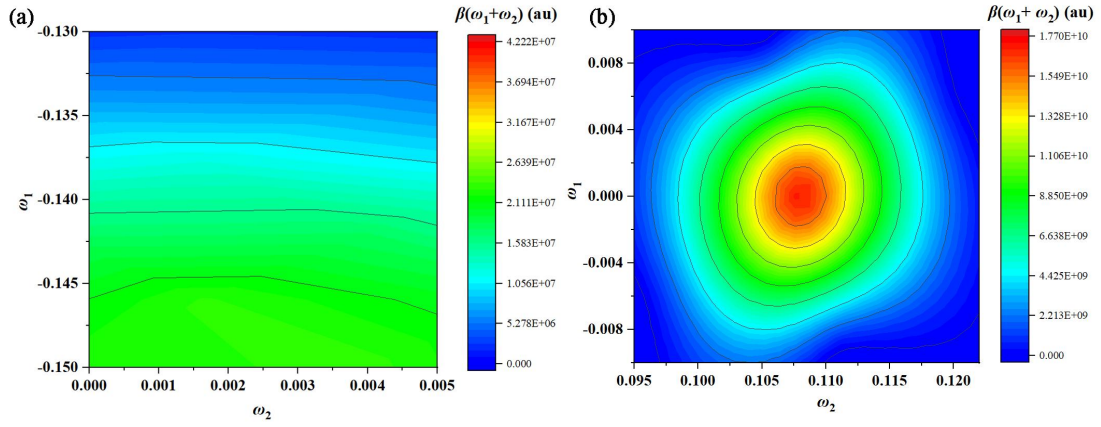
Figure S5. Evolutions of the 2D second-order NLO spectra the [9]HBNG ((a) $F_z = 0$ au, (b) $F_z = 100 \times 10^{-4}$ au).
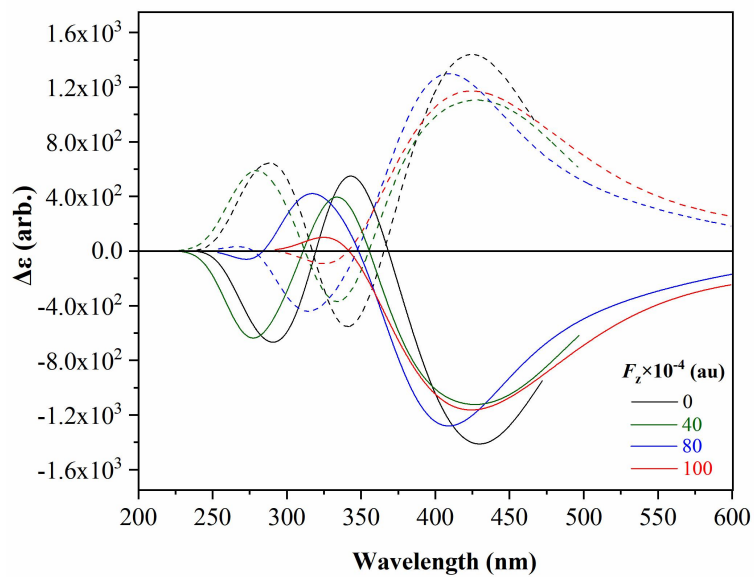
Figure S6. Evolutions of the electron circular dichroism (ECD) spectrum of the [9]HBNG under the F_z ($F_z = 1 \times 10^{-4}$, au).

Table S1. Evolutions of the β_x, β_y, β_z and β_{tot} values of [9]HBNG under the vertical F_z ($F_z = 1 \times 10^{-4}$, au).

$F_z = 1 \times 10^{-4}$ (au)	β_x	β_y	β_z	β_{tot}
0	653	0	0	653
20	654	143	538	859
40	670	337	1121	1349
60	689	584	2028	2219
80	707	1011	4369	4540
100	1023	1603	12434	12579