Supporting Information

The dynamical temporal behaviors of guanine-cytosine coherent charge transfer

Lixia Zhu[1], Qiao Zhou[1], Yongfeng Wan[1], Qi Li[1], Yu Wan[1], Hang Yin[1] and Ying Shi*[1]

[1]Institute of Atomic and Molecular Physics, Jilin University, Changchun 130012, China

Email: shi_ying@jlu.edu.cn

Test calculations on the donor-acceptor complex using different functionals and basis sets to assess the validity of the computational approach used.

Table S1 With the same basis set (TZVP), the maximum absorption peak of G-C was calculated by different functionals.

	B3LYP	CAM-B3LYP	PBEPBE	mPW1PW191	ωB97XD	Exp[a].
G-C	259 nm	221 nm	344 nm	235 nm	221 nm	260 nm

Table S2 With the same functional (B3LYP), the maximum absorption peak of G-C was calculated using different basis sets.

	TZVP	6-311++G (d)	6-31G (d,p)	cc-pVTZz	aug-cc-pVTZ	Exp[a].
G-C	259 nm	258 nm	251 nm	252 nm	262 nm	260 nm

a Literature: [Miannay et al. *J. Am. Chem. Soc*., 2007, 129, 14574-14575], [Lin et al. *J. Phys. Chem. B.,* 2015, 119, 25, 7994-8000] and [Banyasz et al. *Phys. Chem. Chem. Phys*., 2018, 20, 21381].

Table S3 The oscillator strengths (*f*) of G-C under different excited states (B3LYP/TZVP).

	S_1	S_2	S_3	S_4	S_5
f	0.0016	0.0082	0.0002	0.0959	0.0336

Table S4 The energy of photoexcitation from HOMO to LUMO+2 (B3LYP/TZVP).

	HOMO	LUMO	LUMO+1	LUMO+2
Energy (a.u.)	0.185	0.043	0.007	0.010