

Supporting Information

Influence of Nitrogen Doping on Vacancy-Engineered T-Graphene Fragments: Insights into Electronic and Optical Properties

Jyotirmoy Deb,^{a,*} and Pratim Kumar Chattaraj^{b,*}

^a *Materials Science Group, Coal, Energy and Materials Sciences Division, CSIR-North East Institute of Science and Technology, Jorhat 785006, Assam, India*

^b *Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi 835215, Jharkhand, India*

*Email: deb.jyotirmoy11@gmail.com (J.D.)

pratim.chattaraj@gmail.com (P.K.C.)

Table S1. Electrostatic component (E_{elec}), steric component (E_{ster}), quantum component (E_{quan}) and total energy (E) of TF, vacancy-induced TF and NTFs

System	E_{elec} (eV)	E_{ster} (eV)	E_{quan} (eV)	E (eV)
TF	-54067.448	23507.196	1854.016	-28706.237
v-TF	-46462.990	20243.147	1543.261	-24676.581
v-NTF1	-49929.450	21509.619	1937.762	-26482.069
v-NTF2	-49919.202	21501.360	1943.602	-26474.240
v-NTF3	-49929.606	21513.254	1934.558	-26481.793
v-NTF4	-53378.404	22756.582	2347.173	-28274.649
v-NTF5	-53389.166	22764.046	2341.626	-28283.493

Table S2. Static and frequency-dependent polarizabilities of vacancy-induced TF and NTFs

Systems	$\alpha(0;0)$ (au)	$\alpha(\omega;\omega)$ (au)	
		$\omega = 0.0428$ au	$\omega = 0.0856$ au

v-TF	355.562	389.446	391.755
v-NTF1	338.305	353.442	422.475
v-NTF2	388.543	413.057	409.631
v-NTF3	318.336	331.494	396.654
v-NTF4	315.907	326.424	369.442
v-NTF5	270.052	275.763	296.738

Table S3. First-order static and frequency-dependent hyperpolarizabilities of vacancy-induced TF and NTFs

Systems	$\beta(0;0,0)$ (au)	$\beta(-\omega;\omega,0)$ (au)		$\beta(-2\omega;\omega,\omega)$ (au)	
		$\omega = 0.0428$ au	$\omega = 0.0856$ au	$\omega = 0.0428$ au	$\omega = 0.0856$ au
v-TF	0.037	19.254	780.260	1.183	7.066
v-NTF1	0.058	9.356	80.385	0.305	58.170
v-NTF2	1228.048	11033.623	1521.465	4678.391	782184.422
v-NTF3	1.374	2.136	55.867	2.475	204.944
v-NTF4	162.629	178.125	246.319	215.940	16641.588
v-NTF5	0.049	1.341	9.893	0.110	12.837

Table S4. Second-order static and frequency-dependent hyperpolarizabilities of vacancy-induced TF and NTFs

Systems	$\gamma(0;0,0,0)$ (au) $\times 10^4$	$\gamma(-\omega; \omega,0,0) \times 10^4$ (au)		$\gamma(-2\omega; \omega, \omega,0) \times 10^4$ (au)	
		$\omega = 0.0428$ au	$\omega = 0.0856$ au	$\omega = 0.0428$ au	$\omega = 0.0856$ au
v-TF	37.797	77.953	2379.332	-142.067	896.480
v-NTF1	21.424	27.348	60.582	40.814	-299.347

v-NTF2	36.565	-4.756	-36.871	-1.173	12066.331
v-NTF3	20.631	26.792	50.662	36.184	-71.451
v-NTF4	18.673	21.967	43.146	31.466	3161.48812
v-NTF5	9.906	11.162	17.238	14.770	-207.2868
