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

SUPPORTING INFORMATION

New Two-dimensional Carbon Nitride Allotrope with 1:1 Stoichiometry Featuring Spine-like structures: A Structural and Electronic DFT-D Study

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Figure S1. tri-s-triazine based structure of g-C_3N_4 allotrope tested structure with Phonon spectra.

Figure S2. s-triazine based structure of g-C_3N_4 allotrope tested structure with Phonon spectra.

Figure S3. g-C_3N_3 tested structure with Phonon spectra.

Figure S4. Cubic gauche-CN tested structure with Phonon spectra.

Figure S5. Displayed bondlengths of predicted CN allotrope.

Figure S6. BOMD simulation of new CN allotrope.

Figure S7. Comparison of Band structure calculations by using PBE and HSE06 functionals.

Data 1. Cell parameter and fractional XYZ coordinates of new predicted structure.

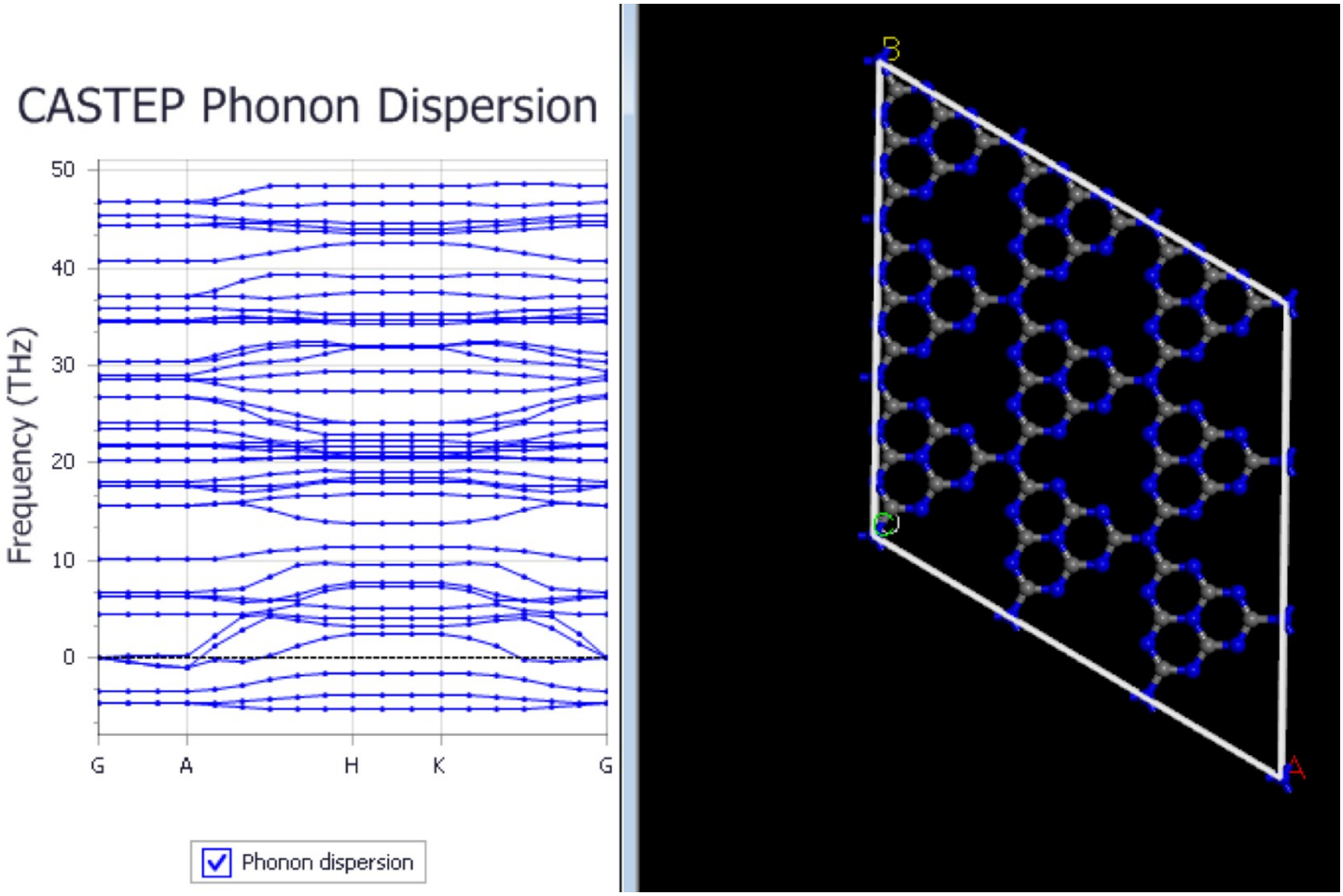

Figure S1. tri-s-triazine based structure of g-C_3N_4 allotrope tested with Phonon spectra. This allotrope is currently used and accepted as representing g-C_3N_4. This was introduced in paper by kroke et al. Reference 9. **From our calculations**, this allotrope is not expected as a candidate to represent this 3:4 stoichiometry because of featured imaginary frequencies along all the path of k-points used to sample the first Brillouin Zone. It has a band gap of **1.21 eV** (GGA/PBE approach).

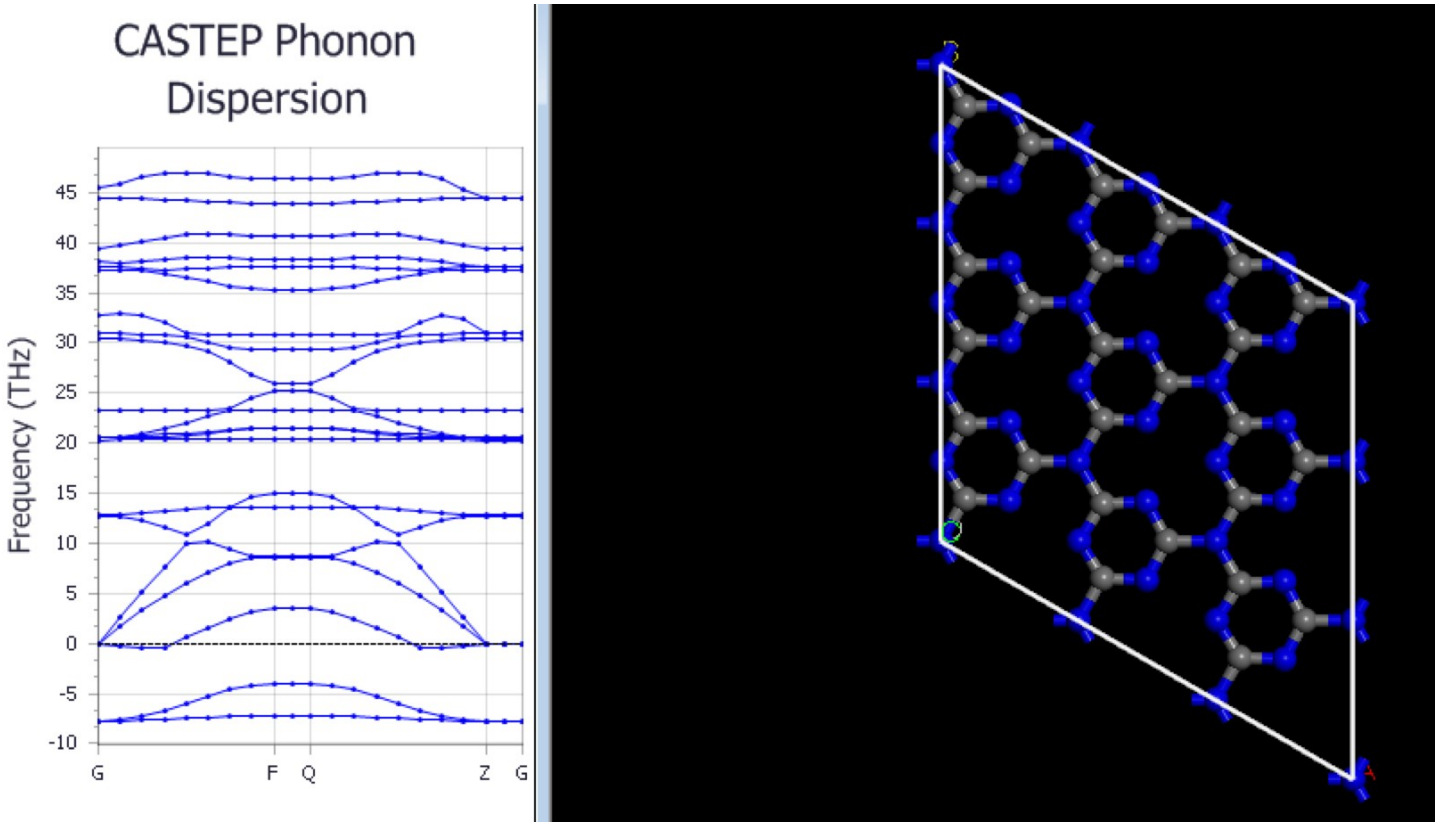

Figure S2. s-triazine based structure of g-C_3N_4 allotrope tested with Phonon spectra. Clearly, this allotrope can not be expected as a candidate to represent g-C_3N_4. Imaginary frequencies are found along all the path of k-points used to sample the first Brillouin Zone. Calculated GGA/PBE band gap was of 1.62 eV.

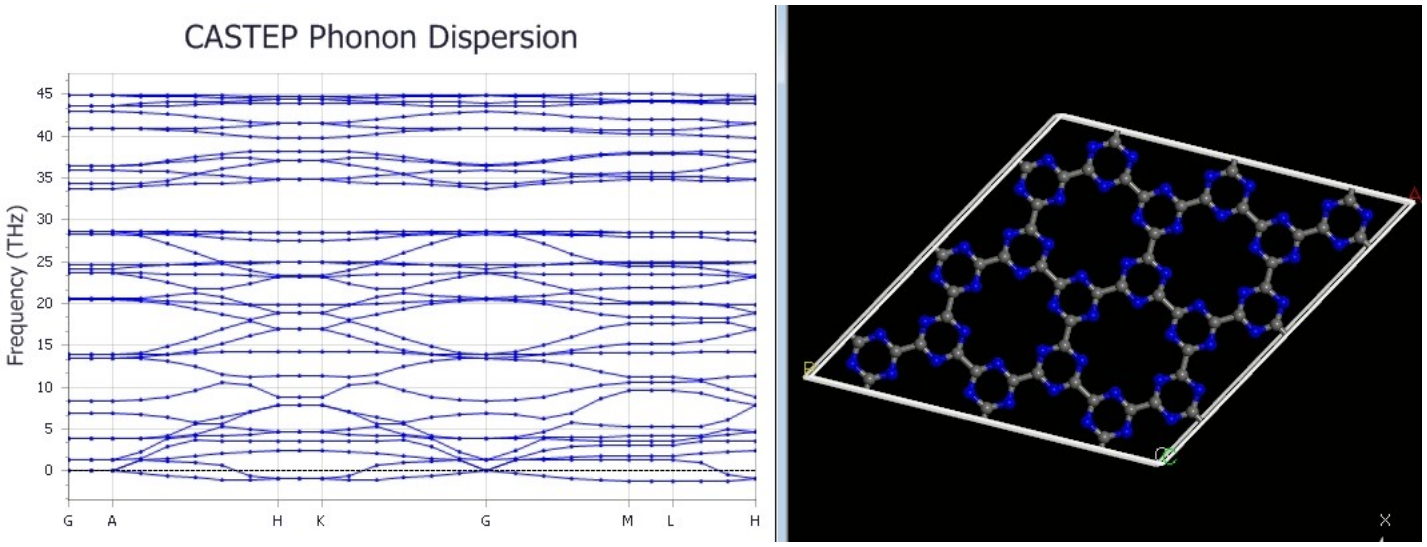

Figure S3. Structure of g-C_3N_3 allotrope tested with Phonon spectra. It holds imaginary frequencies along all the path of k-points used to sample the first Brillouin Zone. This structure was studied by Ma et al. in reference 11. Calculated GGA/PBE band gap was of 1.53 eV.

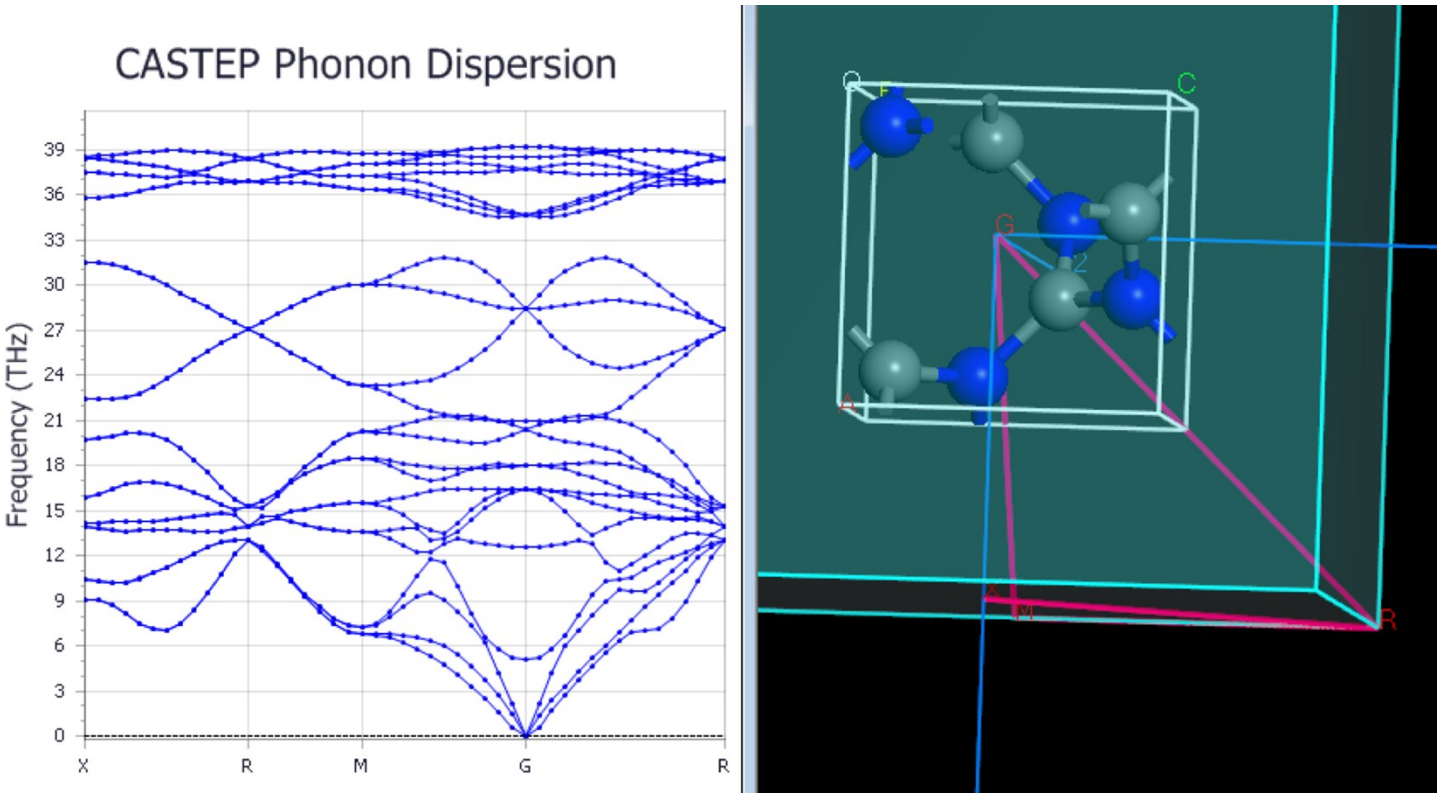

Figure S4. Cubic gauche-CN structure tested with Phonon spectra. This structure was studied by Wang et al. in reference 7. From the calculated phonon dispersion curve lacking of imaginary frequencies, is straight to expect it in experimental samples. The calculated GGA/PBE band gap reveals it as metallic.

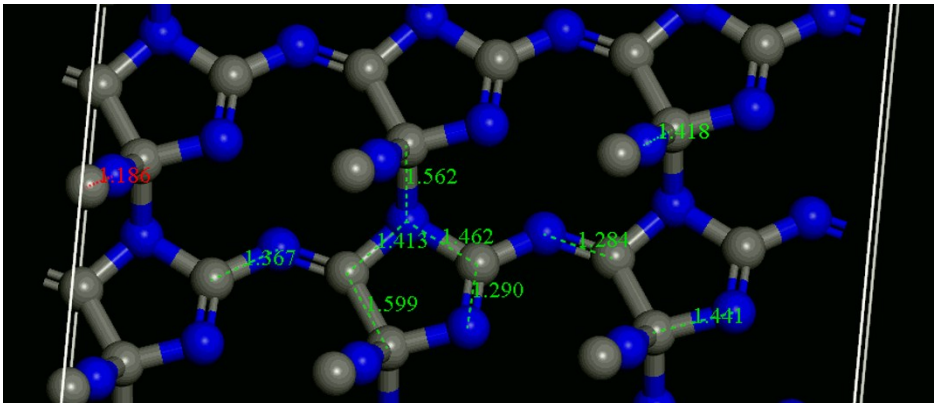

Figure S5. Displayed bond lengths of predicted CN allotrope. A (3x3) supercell is displayed.

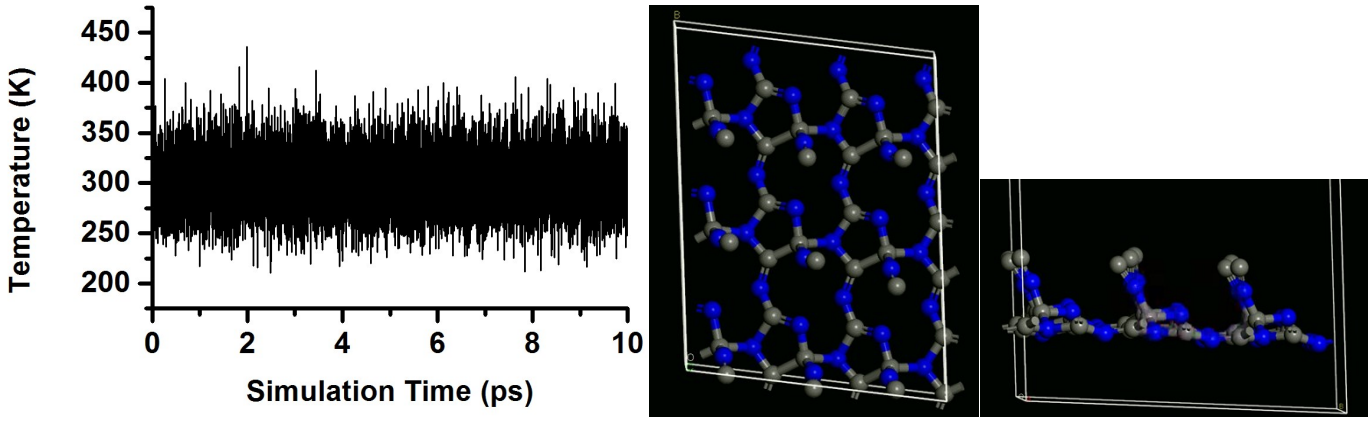

Figure S6. BOMD simulation of new CN allotrope. Total time of simulation was of 10 ps with both temperature (300 K) and pressure (1 atm) controlled. The structure is stable at 300 K it is not disrupted and no surface reconstruction is obtained.

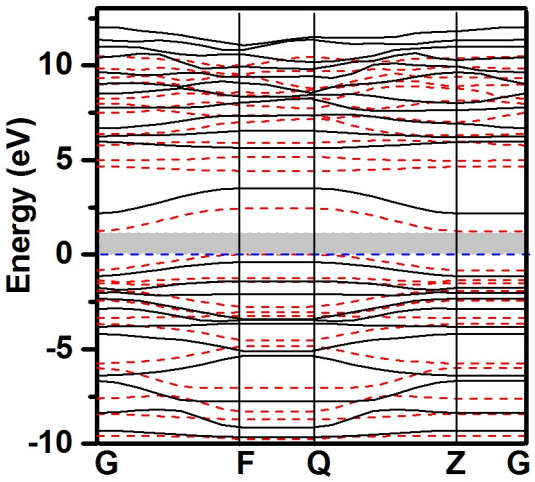

Figure S7. Comparison of Band structure calculations by using PBE (dotted lines) and hybrid HSE06 xc functionals.

Cell parameter of unit cell of new CN allotrope (GGA/PBE)

Unit Cell

Real Lattice(A)			Reciprocal Lattice(1/A)		
3.4936004	-0.6060078	-0.1007414	1.7918765	-0.0346596	-0.0206553
0.0871556	4.6570613	-0.2536846	0.2338706	1.3456494	0.0156477
0.2243258	-0.2705623	19.9146242	0.0120437	0.0169664	0.3156009

Lattice parameters(A)		Cell Angles	
a =	3.547201	alpha =	93.883364
b =	4.664780	beta =	90.858477
c =	19.917725	gamma =	98.662423

Current cell volume = 324.963312 A**3

x	Element	Atom Number	Fractional coordinates of atoms u	v	w	x
x	C	1	0.381799	0.193459	0.189657	x
x	C	2	0.997329	0.012306	0.156688	x
x	C	3	-0.009717	0.502830	0.164383	x
x	C	4	0.507831	0.001394	0.306407	x
x	N	1	0.306077	0.488911	0.196076	x
x	N	2	0.753848	0.221196	0.148058	x
x	N	3	0.856692	0.743647	0.143988	x
x	N	4	0.457470	0.093592	0.253469	