Supplementary Information

Structural investigation of graphitic carbon nitride *via* XRD and Neutron Diffraction

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ATOMIC COORDINATES

Table S1 Atomic coordinates of the partially polymerized g-C_3N_4. Unit cell parameters: *a* = b = 13.924 Å, *c* = 6.49 Å, α = β = 90 °, γ = 120 °.

Atom	x	y	z
C1	0.6111	0.55555	0.75
C2	0.6111	1.05555	0.75
C3	1.1111	0.55555	0.75
C4	0.6111	0.7222	0.75
C5	0.6111	1.2222	0.75
C6	1.1111	0.7222	0.75
C7	0.6111	0.88889	0.75
C8	0.6111	1.38889	0.75
C9	1.1111	1.38889	0.75
C10	0.77777	1.38889	0.75
C11	1.27777	0.88889	0.75
C12	1.27777	1.38889	0.75
C13	0.94443	1.38889	0.75
C14	1.44443	0.88889	0.75
C15	1.44443	1.38889	0.75
C16	0.94443	0.55555	0.75
C17	1.44443	0.55555	0.75
C18	1.44443	1.05555	0.75
H1	1.12644	1.25287	0.75
H2	1.12644	0.87356	0.75
H3	0.74711	0.87356	0.75
N1	0.5	0.5	0.75
N2	0.5	1	0.75
N3	1	0.5	0.75
N4	0.5	0.66667	0.75
N5	0.5	1.16667	0.75
N6	1	0.66667	0.75
N7	0.5	0.83333	0.75
N8	0.5	1.33333	0.75

N9	1	1.33333	0.75
N10	0.66667	0.5	0.75
N11	0.66667	1	0.75
N12	1.16667	0.5	0.75
N13	0.66667	0.83333	0.75
N14	0.66667	1.33333	0.75
N15	1.16667	0.83333	0.75
N16	1.16667	1.33333	0.75
N17	0.83333	0.5	0.75
N18	1.33333	0.5	0.75
N19	1.33333	1	0.75
N20	0.66667	0.66667	0.75
N21	0.66667	1.16667	0.75
N22	1.16667	0.66667	0.75
N23	0.83333	1.33333	0.75
N24	1.33333	0.83333	0.75
N25	1.33333	1.33333	0.75

Table S2 Atomic coordinates of the modified Melon with closer chains. Unit cell parameters: *a* = 16.4 Å, b = 12.4 Å, *c* = 6.49 Å, α = β = γ = 90 °.

Atom	x	y	z
C1	0.3448	0.472	0.25
C2	0.6552	0.528	0.25
C3	0.22159	0.798	0.25
C4	0.77841	0.202	0.25
C5	0.26945	0.63	0.25
C6	0.73055	0.37	0.25
C7	0.13605	0.648	0.25
C8	0.86395	0.352	0.25
C9	0.98716	0.683	0.25
C10	0.01284	0.317	0.25
C11	0.07292	0.82	0.25
C12	0.92708	0.18	0.25
C13	0.83442	0.028	0.25
C14	0.16558	0.972	0.25
C15	0.7112	0.702	0.25
C16	0.2888	0.298	0.25
C17	0.75906	0.87	0.25
C18	0.24094	0.13	0.25
C19	0.62567	0.852	0.25
C20	0.37433	0.148	0.25
C21	0.47801	0.817	0.25
C22	0.52199	0.183	0.25
C23	0.56253	0.68	0.25

C24	0.43747	0.32	0.25
H1	0.87494	0.8891	0.25
H2	0.12506	0.1109	0.25
H3	0.38533	0.6109	0.25
H4	0.61467	0.3891	0.25
H5	0.91649	0.5576	0.25
H6	0.08351	0.4424	0.25
H7	0.40734	0.9424	0.25
H8	0.59266	0.0576	0.25
H9	0.35826	0.8217	0.25
H10	0.64174	0.1783	0.25
H11	0.86741	0.6783	0.25
H12	0.13259	0.3217	0.25
N1	0.14216	0.762	0.25
N2	0.85784	0.238	0.25
N3	0.08819	0.935	0.25
N4	0.91181	0.065	0.25
N5	0.22668	0.904	0.25
N6	0.77332	0.096	0.25
N7	0.28269	0.733	0.25
N8	0.71731	0.267	0.25
N9	0.19817	0.588	0.25
N10	0.80183	0.412	0.25
N11	0.05765	0.608	0.25
N12	0.94235	0.392	0.25
N13	0.99734	0.788	0.25
N14	0.00266	0.212	0.25
N15	0.3336	0.568	0.25
N16	0.6664	0.432	0.25
N17	0.92097	0.638	0.25
N18	0.07903	0.362	0.25
N19	0.63178	0.738	0.25
N20	0.36822	0.262	0.25
N21	0.57781	0.565	0.25
N22	0.42219	0.435	0.25
N23	0.71629	0.596	0.25
N24	0.28371	0.404	0.25
N25	0.7723	0.767	0.25
N26	0.2277	0.233	0.25
N27	0.68778	0.912	0.25
N28	0.31222	0.088	0.25
N29	0.54726	0.892	0.25
N30	0.45274	0.108	0.25
N31	0.4882	0.712	0.25

N32	0.5118	0.288	0.25
N33	0.82321	0.932	0.25
N34	0.17679	0.068	0.25
N35	0.41182	0.862	0.25
N36	0.58818	0.138	0.25

Table S3 List of the key parameters for the investigated structural models. Fully polymerized structures are indicated with "f.p.", while partially polymerized structure with "p.p.".

Structure		Cell geometry	a (Å)	b (Å)	c (Å)	α, β, γ (°)	$(210)_{ortho}$ or $(100)_{hexa}$ 2θ (°)	Δ2θ (°)	I_{210}/I_{002} I_{100}/I_{002}
g-C_3N_4	-	-	-	-	-	-	*13.00*	-	*0.19*
Teter & Hemley	f.p.	hexagonal	4.7420	4.7420	6.7205	90, 90, 120	21.62	8.62	0.11
Tri-*s*-triazine	f.p.	hexagonal	7.1130	7.1130	6.4900	90, 90, 120	14.38	1.38	0.18
Döblinger	p.p.	hexagonal	12.77	12.77	6.49	90, 90, 120	8.00	5.00	2.05
Tri-*s*-triazine	p.p.	hexagonal	13.9246	13.9246	6.49	90, 90, 120	7.18	5.82	1.64
Lotsch	p.p.	orthorhombic	16.7	12.4	6.49	90, 90, 90	12.78	0.22	0.44
Melon	p.p.	orthorhombic	16.4	12.4	6.49	90, 90, 90	12.94	0.06	0.37
α = 98 °	p.p.	orthorhombic	16.4	12.4	6.567	98, 90, 90	12.98	0.02	0.38
β = 98 °	p.p.	orthorhombic	16.4	12.4	6.567	90, 98, 90	13.04	0.04	0.36
Shift A	p.p.	orthorhombic	16.4	12.4	6.49	90, 90, 90	12.94	0.06	0.16
Shift B	p.p.	orthorhombic	16.4	12.4	6.49	90, 90, 90	12.94	0.06	0.30
Shift C	p.p.	orthorhombic	16.4	12.4	6.49	90, 90, 90	12.94	0.06	0.33

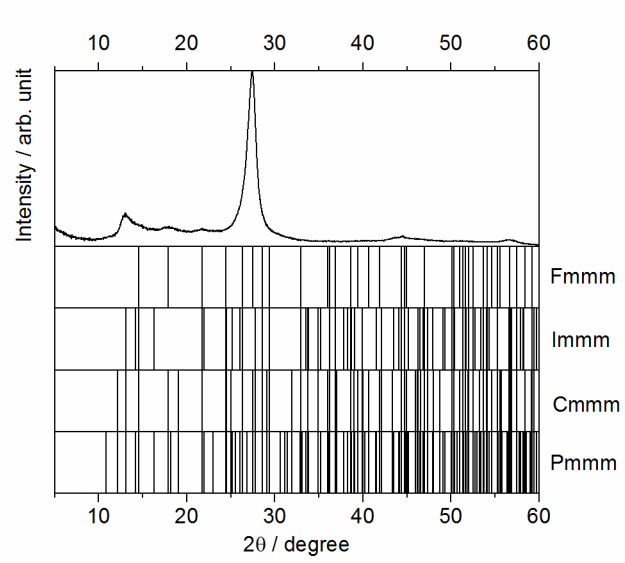

Figure S1 Results of the indexing of the experimental XRD pattern.

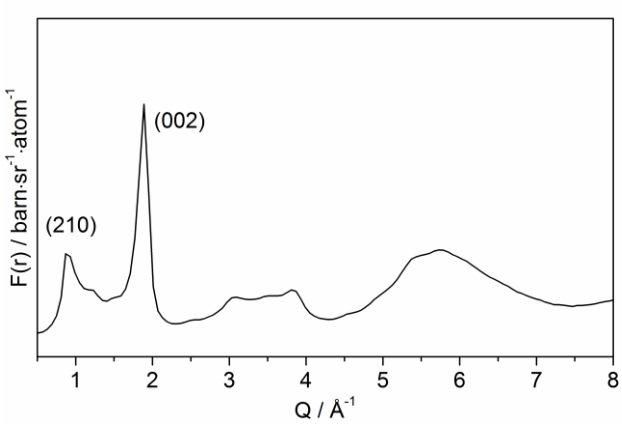

Figure S2 Structure factor of graphitic carbon nitride.

Table S4 Summary of the normalized peak areas as obtained from the Gaussian fitting of the D(r) plots.

	A_{peak}/A_{II}				
r (Å)	C_3N_4	α = 92 °	α = 95 °	β = 92 °	β = 95 °
1.03	0.07	0.15	0.15	0.16	0.15
2.07	0.14	0.09	0.09	0.09	0.09
2.1	1.25	1.23	1.23	1.23	1.22
2.72	0.14	0.12	0.12	0.12	0.12
3.52	0.63	0.66	0.66	0.67	0.65
4.03	0.59	0.68	0.66	0.65	0.67
4.62	0.77	0.41	0.52	0.40	0.49
5.14	0.20	0.06	0.02	0.08	0.04
Rw	-	0.41	0.41	0.41	0.41

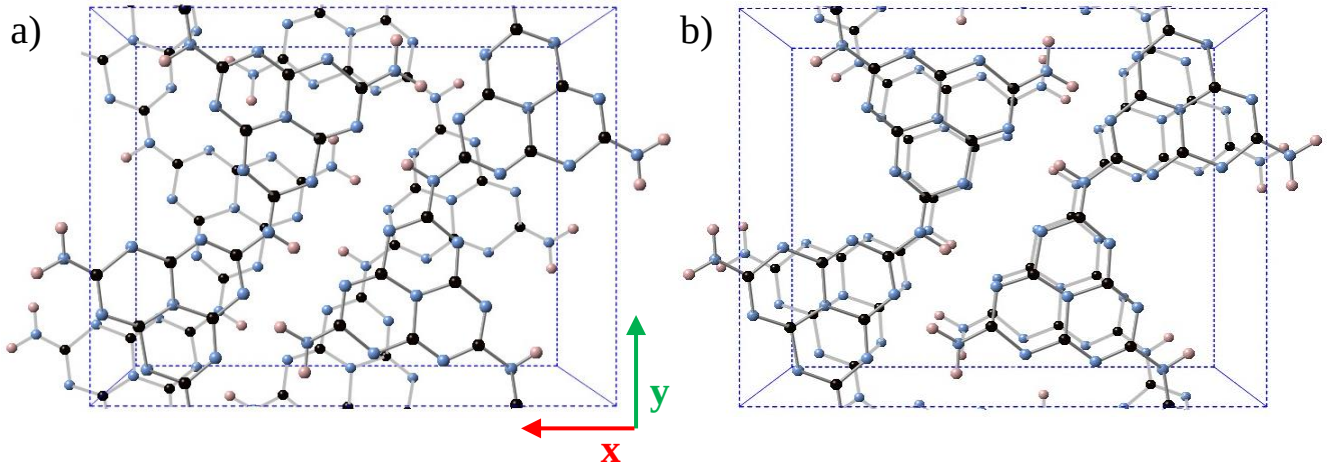

Figure S3 Representation of the crystal structure of a) modified Melon with randomly shifted layers and b) original modified Melon.