Electronic Supplementary Material (ESI) for RSC Advances

In situ Raman Spectroscopy and Thermal Analysis of the Formation of Nitrogen-Doped Graphene from Urea and Graphite Oxide

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Supplementary Information

Figure S1 shows the original Raman spectra of the graphite oxide/urea (1:1) mixture in comparison with the as-produced graphite oxide (GO) and pristine urea. The Raman spectrum of GO exhibits broadened D and G bands and is subject to a broad luminescent background. These features are also observed in the GO/Urea sample. The most pronounced Raman feature in the spectrum of urea is a strong peak around ~1010 cm^{-1}. However, the peak does not appear in the Raman spectrum of the GO/urea mixture, suggesting that Raman signal of GO is significantly stronger than that of the urea compound.

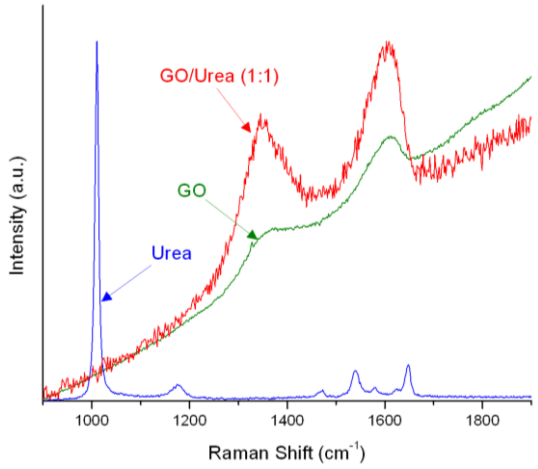

Figure S1: Raman spectra of urea, graphite oxide (GO), and a GO/urea (1:1) mixture, recorded using 514 nm laser excitation.

Table S1 show the results from the curve fitting of the D and G band in the Raman spectra of a GO/urea mixture (1:1) and the exfoliated graphene. Peak fitting was performed after baseline correction using Renishaw's Wire2.0 Raman software.

Table S1: Curve fitting data of D and G Raman bands.

Peak [unit]	**Position [cm^{-1}]**	**FWHM [cm^{-1}]**	**Intensity [a.u.]**	**Area [a.u.]**
GO/Urea				
G1	1588.1	91.5	0.75	85.7
D1	1346.3	86.9	0.53	55.4
G2	1617.0	36.7	0.28	10.9
D2	1396.7	262.5	0.43	158.9
Graphene				
D1	1353.2	90.6	0.52	59.8
G2	1550.0	123.0	0.30	48.4
G1	1602.9	67.8	0.72	51.8
D2	1358.5	261.7	0.46	154.2

Figure S2 shows the high-resolution XPS spectra of the C 1s, N 1s, and O 1s energy regions. The peak assignment is based on previous studies on GO/urea-derived and nitrogen-doped graphene (see Ref. 29 and 42 in the manuscript). However, it should be noted that in the presence of different amounts of urea during thermal exfoliation of GO, the surface chemistry of the resulting graphene may change. The exact nature of the functional groups in GO/urea-derived graphene will thus be determined in a follow-up study using a combination of FTIR and XPS measurement.

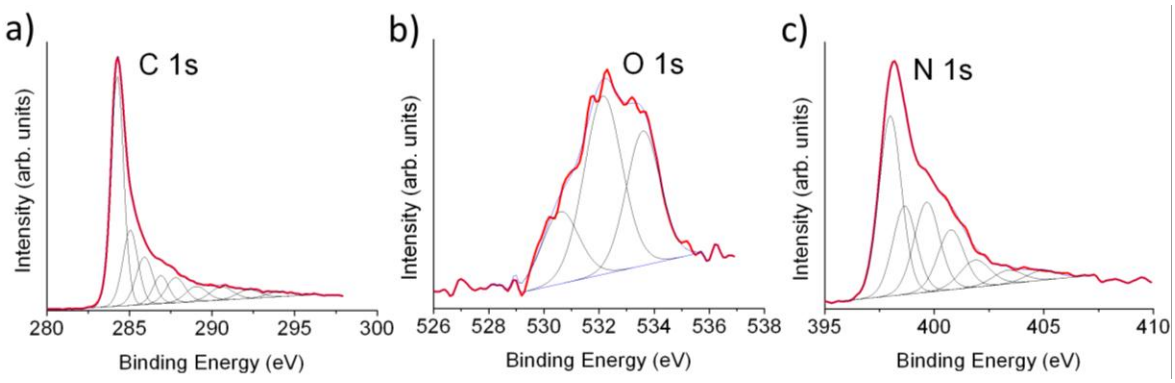

Figure S2: High-resolution XPS spectra of the C1s (a), O1s (b), and N1s (c) energy range of a GO/urea (1:1) sample.

Table S2: Data from XPS analysis of C 1s, N 1s, and O 1s energy peaks.

Assignment	C graphitic	C-C/ C*-CO	C-N	COH/ COC	CNO/ C=O	COOH/ N-C(O)O	Not assigned
Energy (eV)	*284.3*	*285.2*	*285.9*	*286.8*	*287.8*	*289.1*	*>290.6*
Graphene (thermal)	49.6%	12.1%	10.6%	5.1%	6.6%	5.8%	10.3%
Graphene (urea)	42.7%	17.6%	11.1%	6.7%	7.6%	4.7%	9.6%

Assignment	imine	NH_2CO	amine	N-(C=O)2	NH3+	N oxides
Energy (eV)	*398.0*	*398.7*	*399.7*	*400.8*	*401.9*	*>403.4*
Graphene (thermal)	-	-	-	-	-	-
Graphene (urea)	34.6%	19.0%	19.9%	13.1%	6.5%	7%

Assignment	O=N-C	N-C=O	C-O-NO2/ C-O
Energy (eV)	*530.9*	*532.2*	*533.6*
Graphene (thermal)	25.0%	12.4%	62.5%
Graphene (urea)	22.2%	41.0%	36.8%