Supplementary Materials



Figure S1. Scanning electron microscope pictures showing the morphology of (a) pristine nanodiamonds showing loosely bound agglomerates and (b) carbon onion showing tightly bound aggregates reaching several micrometers in size.



Figure S2. Raman spectra of ND and OLC showing the F2g peak corresponding to the sp³ diamond at 1325 cm⁻¹, D band and G band corresponding to sp² disorder at ~ 1330 cm⁻¹ and ~1570 cm⁻¹, respectively. Post annealing, OLC spectra consists of a broad D band in the region 1332-1350 cm⁻¹, attributed to increase in the sp² disorder with a background of sp³ diamond, indicating the transformation of diamond to graphite [29].

Table S1. Raman shifts, areal intensities and peak widths obtained from the spectra of ND and OLC determined by fitting spectra with a Gaussian line shape using Origin software. After annealing, the FWHM of G band decreased, suggesting the formation of graphitic shells [30–32].

Sample	Peak Position (cm ⁻¹)	FWHM ^a (cm ⁻¹)	Peak Assignment	
ND	1325	189.7	Diamond	
	1594	116.4	G-sp ² dimers	
OLC	1343	204	D-Graphite	
	1587	89	G-Graphite	

^a Peak Full width at half maximum.



Figure S3. XPS spectra of pristine nanodiamonds showing an intense carbon peak at 284 eV and two weak nitrogen and oxygen peaks at 400 and 532 eV, respectively. (a) and carbon onion showing a decrease in intensity for carbon, oxygen and nitrogen peaks (b). The major peaks are marked for Carbon (C 1s), Nitrogen (N 1s) and Oxygen (O 1s) present on the surface.



Figure S4. XPS C KLL Auger Spectra (a) and their first derivatives (b) as compared with pristine nanodiamonds (ND) and carbon onion (OLC). D parameter represents the width between maximum and minimum excursions of the derivative of Auger spectra. D value was found to increase after annealing, indicating an increase in the content of sp2 carbon [28].

Table S2. The relative atomic contents of carbon, oxygen, and nitrogen, and the relative atomic contents of different chemical states of carbon determined from XPS analysis. The atomic percentage of carbon increased, while the atomic percentage of nitrogen and oxygen decreased post annealing, which could be due to the reduction in the surface dangling bonds, such as –C-H and –C-O- bonds, during annealing [28]. After annealing, the sp² content was found to increase to 68%, indicating the conversion of diamond to graphite and OLC still contains 32% of sp³ carbon, indicating the presence of diamond core.

Sample	C (%)	0 (%)	N (%)	C KLL Auger spectra		
				D ^a (eV)	Sp² (%)	Sp ³ (%)
ND	93.8	3.9	1.9	13	0	100
OLC	97.1	1.6	1.0	19.1	68	32

^a D parameter represents the width between maximum and minimum excursions of the derivative of Auger spectra.



Figure S5. XRD patterns of PA showing typical diffraction peaks of crystalline PA (15.4°, 18.1°, 20.3°, 23.3°, 24.2° and 26.4°(20), [44]).



Figure S6. XRD patterns of ibuprofen showing typical diffraction peaks of crystalline IBU (16.4°, 17.4°, 20° and 22° (20), [45,46]).