

# Synthesis and improved emission characteristics of BCNO@silica composite

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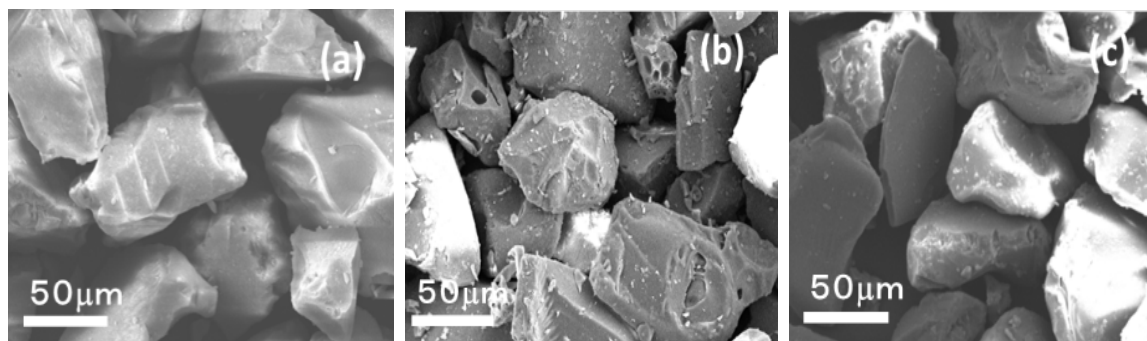
## Electronic supplementary information (ESI):

### 1. Characterization

Formation of BCNO was confirmed by x-ray diffraction (XRD) [RIGAKU, Ultima IV] using Cu-K $\alpha$  radiation, morphologies of the samples were investigated using scanning electron microscopy (SEM) equipped with EDS [JEOL, JSM-5900 LVS]. Transmission electron microscopy (TEM) and energy electron loss spectroscopy (EELS) were performed using Techni G<sup>2</sup> at 200 keV. Information about the bonding states were extracted from x-ray photoemission spectroscopy (XPS) [Perkin-Elmer  $\Phi$  04-500 dual anode x-ray source instrument] and Fourier transform infrared spectroscopy [FTIR-8700, SHIMADZU]. Before recording the XPS data, sample surface was etched by using low energy argon ion gun to remove the surface contaminations. Photoluminescence (PL) and UV-visible spectra were recorded using Hitachi F-4500 fluorescence spectrometer and U-4100 spectrophotometer, respectively. PL decay lifetimes were estimated from the decay profile using 371 nm nano LED [Fluorolog, Horiba Jobin Yvon]. Quantum efficiency of the sample B2 was measured using QE-1100 [Otsuka Electronics] at excitation wavelength range 390-450 nm with 10 nm interval. All the measurements were performed at room temperature.

### 2. Scanning electron microscopy (SEM)

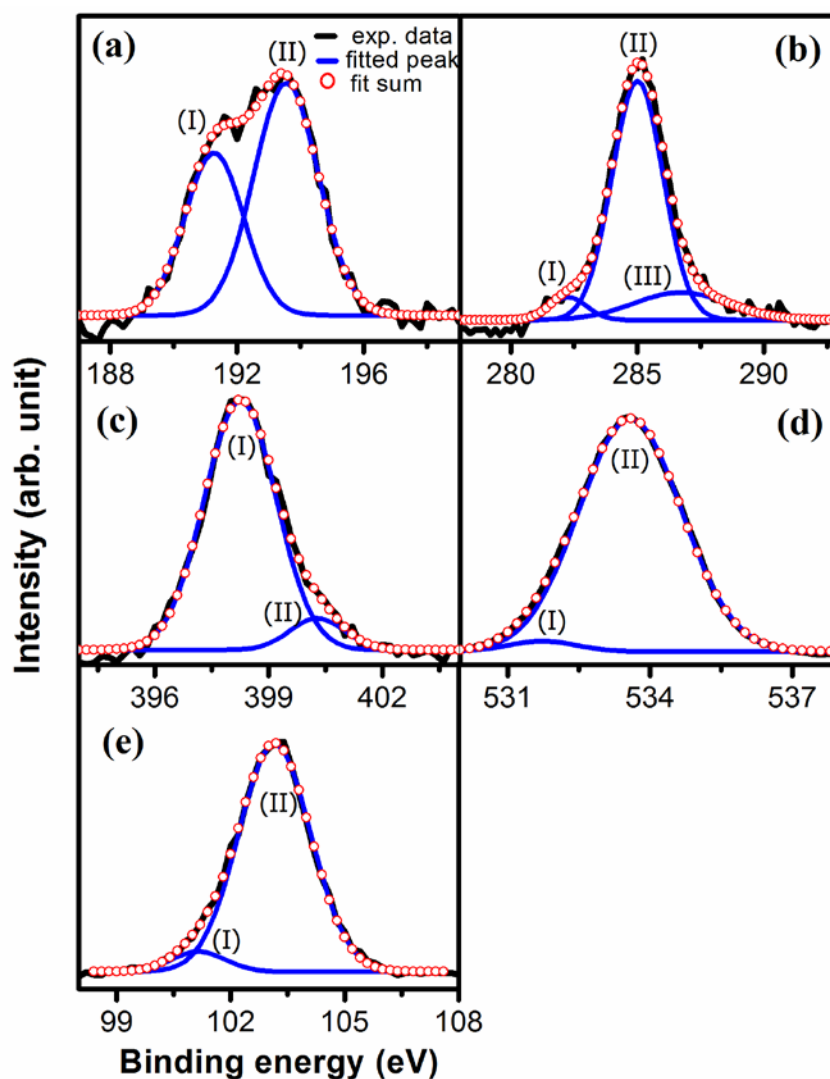
Fig. S1 (a)-(c) represent the SEM micrographs of pure silica particles, sample B2 (as-prepared) and sample B2 after washing by acid, respectively. Identical images (a) and (c) ruled out the presence of surface residuals on the silica particles.



**Fig. S1:** SEM micrographs of (a) Pure silica particles (b) sample B2 (as-prepared) and (c) sample B2 after 30 min. acid wash.

### 3. X-ray photoemission spectroscopy (XPS)

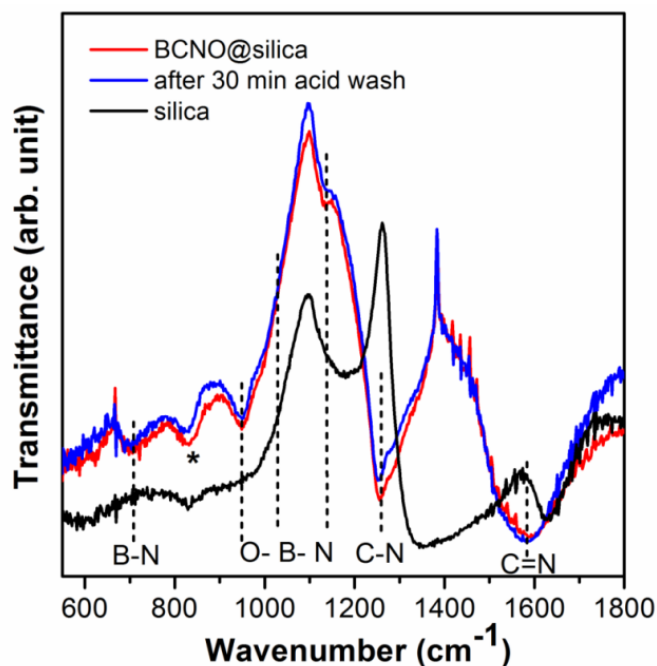
Bonding characteristics and atomic compositions were examined from XPS spectra of B 1s, C 1s, N 1s, O 1s, and Si 2p core level electrons for sample B2, as shown in Fig. S2(a)-(e), respectively. Quantitative elemental analysis gives B/C/N/O/Si ratio of 8/9/4/64/15. Here, the higher percentages for O and Si atoms are because of the SiO<sub>2</sub> matrix. Typical XPS signals were analyzed further, to get the information about bonding characteristics. Fig. S2 (a) shows two peaks (I) and (II) at the positions 191.3 and 193.5 eV, respectively. Peak (I) at 191.3 eV is attributed to the B-N bonding in *h*-BN whereas, peak (II) at higher energy is assigned to the B-O bonding.<sup>1-5</sup> Fig. S2 (b) exhibits three components (I), (II) and (III) at the positions 282.3, 285.0 and 286.7 eV, respectively. These peaks show consistency with the previously reported data for C-B, C-C and C-N bonding in BCN compounds.<sup>1,2</sup> The electronegativity values of B atom is lower than C atom, whereas for N atom, electronegativity is higher than C atom, which results in the shift towards lower and higher binding energies. Fig. S2 (c) shows the typical XPS spectrum for N 1s electrons. An asymmetric peak can be deconvoluted further in to two peaks, positioned at 398.3 and 400.3 eV. Peak (I) at lower energy side is assigned to N-B bonding, whereas peak (II) at higher energy side designated to the N-C bonding.<sup>6</sup> Fig. S2 (d) shows two contributions at 531.7 and 533.6 eV, for O 1s. The lower energy side peak (I) is explained by oxygen substitution for N-B-O and peak (II) at 533.6 eV defined as the characteristic peak for SiO<sub>2</sub>. In the Fig. S2 (e), peak (I) at 101.1 eV is assigned to SiC, whereas peak (II) at 103.1 eV referred to SiO<sub>2</sub>.<sup>7</sup> Thus, it can be concluded that sample B2 is a compound with B-C-N hybridization in mesoporous SiO<sub>2</sub> matrix.



**Fig. S2:** XPS spectrum of (a) B1s (b) C1s (c) N1s (d) O1s and (e) Si-2p for sample B2.

#### 4. Fourier transform infrared spectroscopy (FTIR)

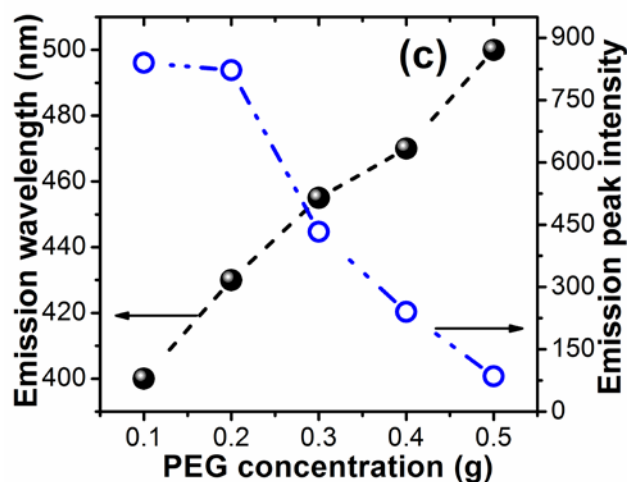
Fig. S3 shows the various IR vibration modes for pure silica and sample B2 (before and after acid wash). The presence of BCN was confirmed by B-N, N-B-O, C-N, and C=N vibrations at  $\sim 705$ , 900-1100, 1253, and 1587  $\text{cm}^{-1}$ , respectively.<sup>8-11</sup> IR mode marked by asterisk was assigned to  $\text{SiO}_2$  matrix. Taking the above results into consideration including XRD, SEM, TEM, EDS and XPS we infer that, BCNO NPs are mainly formed and retained within the mesoporous silica channels.



**Fig. S3:** FTIR spectrum for sample B2.

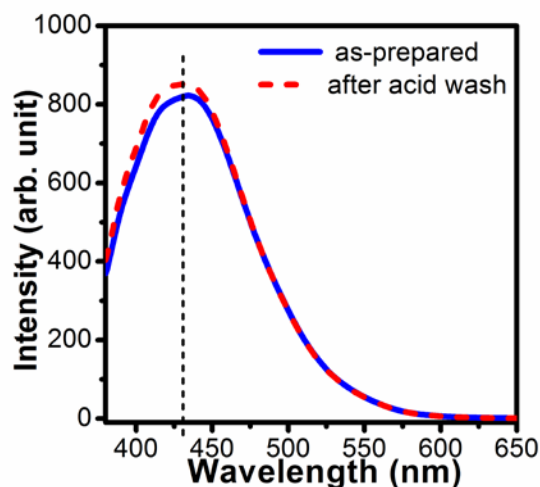
## 5. Photoluminescence

Fig. S4 shows the relation between PEG<sub>200</sub> content, emission wavelength and emission peak intensity. We observed almost linear dependence in the emission wavelength with PEG<sub>200</sub> concentration, moreover PL intensity decreased with increasing amount of carbon concentration.



**Fig. S4:** Graph between emission wavelength and emission peak intensity with respect to PEG<sub>200</sub> concentration

PL intensities of sample B2 remains unaffected before and after acid wash, shows that BCNO@silica composite highly chemically stable.



**Fig S5:** A comparison of PL intensities of sample B2, before and after acid wash.

## References

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