Supplementary Information For:

Metal free alkene hydrogenation by B- doped graphitic carbon nitride

Ashima Dogra, Ilaria Barlocco, Amritpal Singh, Ferenc Somodi, Alberto Villa* and NeerajGupta*

1. Preparation of catalyst

1.1 g- C_3N_4

8g urea was taken in a well dried covered crucible. The contents were heated in muffle furnace for 30 minutes at 450°C. Cooled the contents to room temperature and stored in dried vessel (25-30ºC).

1.2 FBCN

8g urea was taken and 0.8 ml HBF_4 (0.002 moles) was added to it. The contents were heated in muffle furnace for 40 minutes at 450ºC. Cooled the contents to room temperature and stored in dried vessel (25-30ºC).

1.3 OBCN

OBCN was prepared by using 8g urea and aqueous solution of H_3BO_3 (0.002 moles; the boric acid solution was prepared by adding 0.123 g of boric acid in 4 ml distilled water). The contents were heated for 40 minutes at 450ºC. Cooled the contents to room temperature and stored in dried vessel (25-30ºC).

2. Characterization

2.1 SEM-EDX

SEM-EDX spectrum and elemental map of material FBCN in Fig S1 and S2.

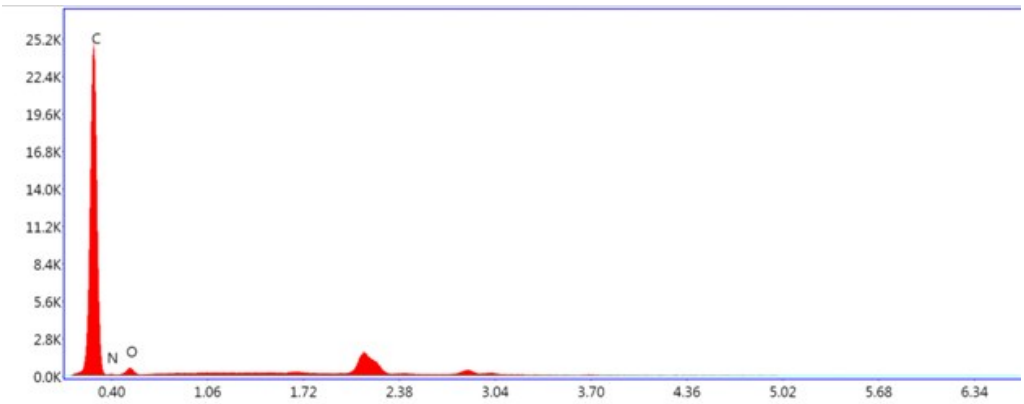

Figure S1. EDX spectrum of FBCN

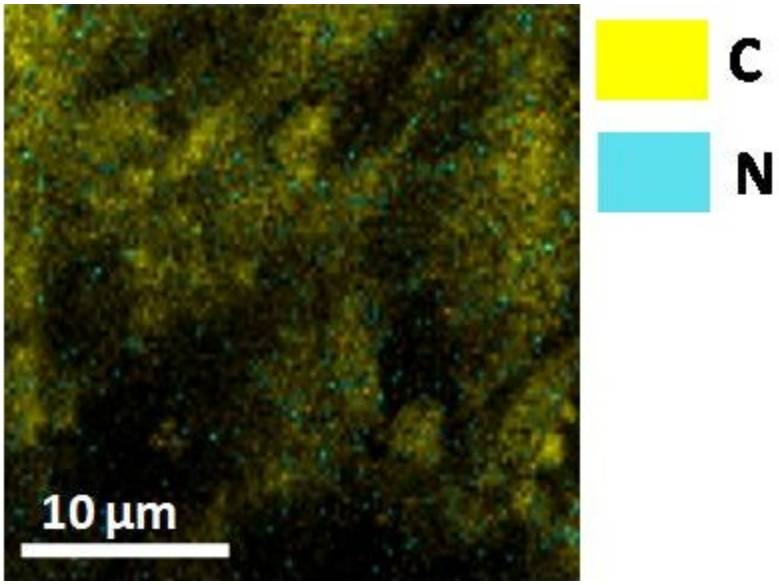

Figure S2. Elemental Map of FBCN showing N species

2.2 FTIR Spectroscopy

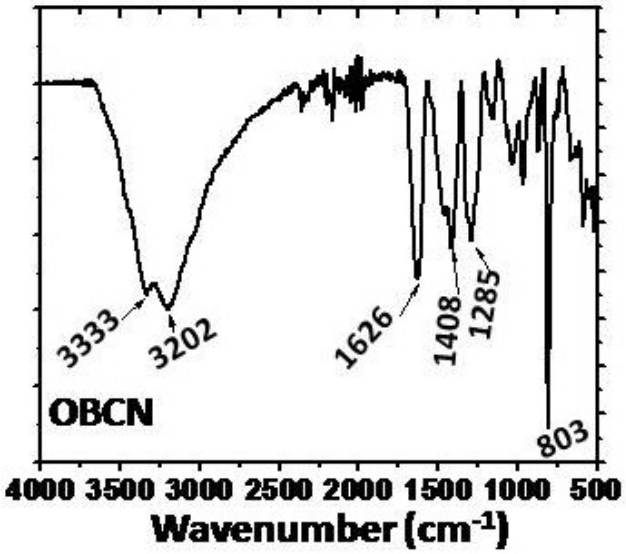

Figure S3. FTIR spectra of OBCN

2.3 Reaction scheme of BN model for DFT calculations

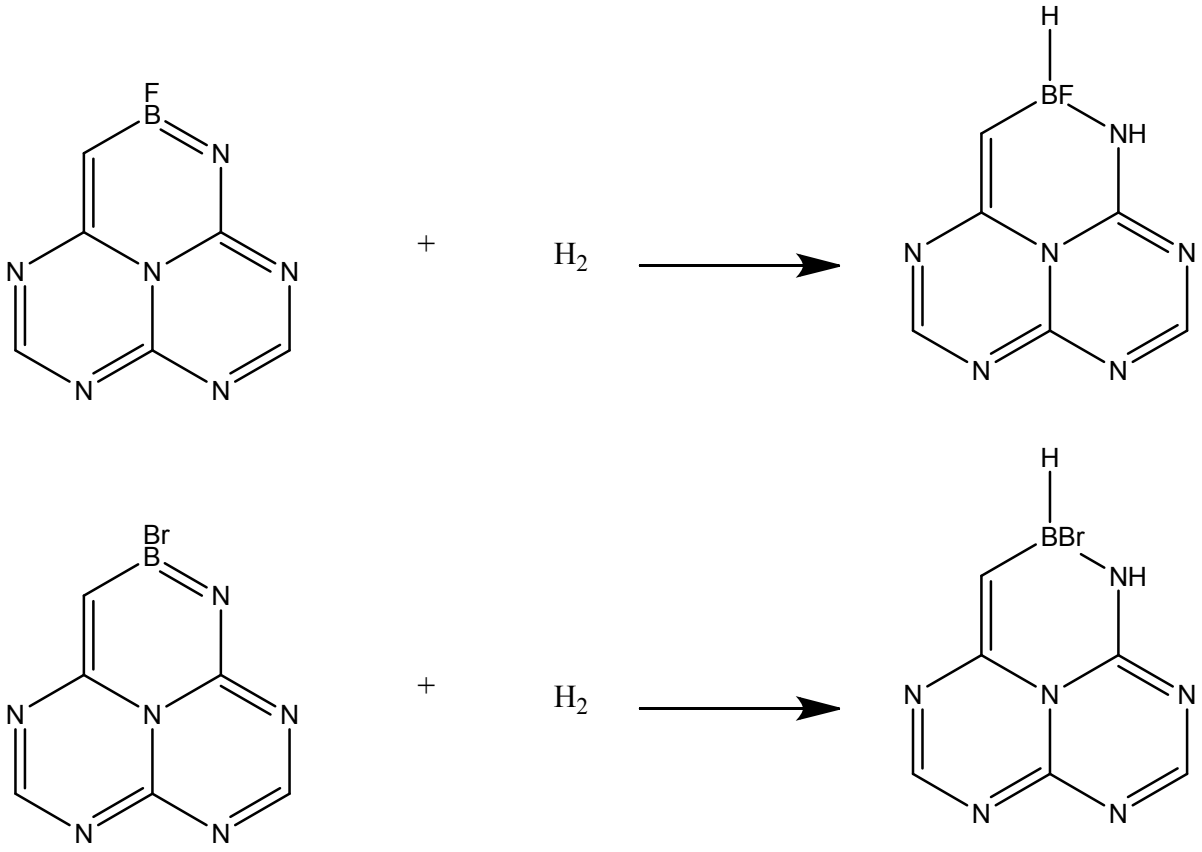

Figure S4. Reaction of model BN molecule containing F and Br atoms with hydrogen molecule

3. Hydrogenation of Styrene

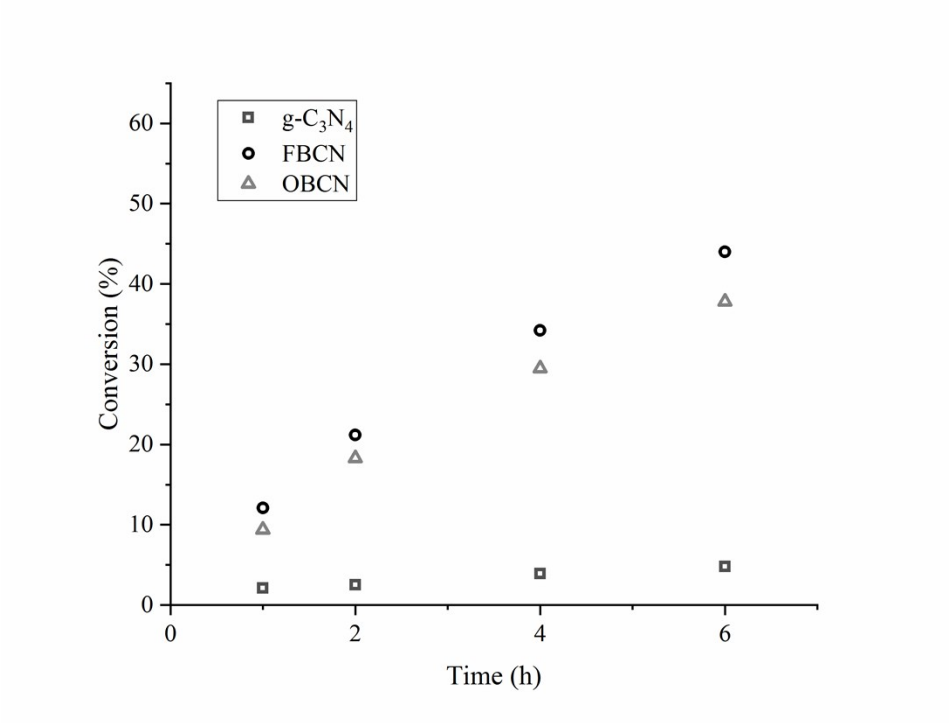

Figure S5. Conversion vs time of g-C3N4, FBCN and OBCN catalysts at 150°C