Impact of electron-phonon coupling, Stokes Shift and quantum confinement in Boron Nitide quantum dots for hydrogen production through water splitting.

Supplementary information

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I. Calculation of Huang-Rhys factor (S)

For the sample S3 (filling volume of 85.7%)

$$E_{stokes} = 2S\hbar\omega[1], [2], [3] \tag{S1}$$

where, $\hbar\omega$ is calculated using,

$$E_{em} = E_{ZPL} - n\hbar\omega[4] \tag{S2}$$

$$n\hbar\omega = E_{ZPL} - E_{em} \tag{S3}$$

where, n is 1, as there is one phonon sideband, hence from Eqn.S3, we get,

$$\hbar\omega = 4.25\,eV - 3.37\,eV$$

$$\hbar\omega = 0.88\,eV$$

Further, from Eqn.S1, we can calculate the S as follows,

$$S = E_{Stokes}/2(\hbar\omega) \tag{S4}$$

$$S = 1.36\,eV/2(0.88\,eV)$$

$$S = 0.772$$

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Fourier Transform Infrared Spectra

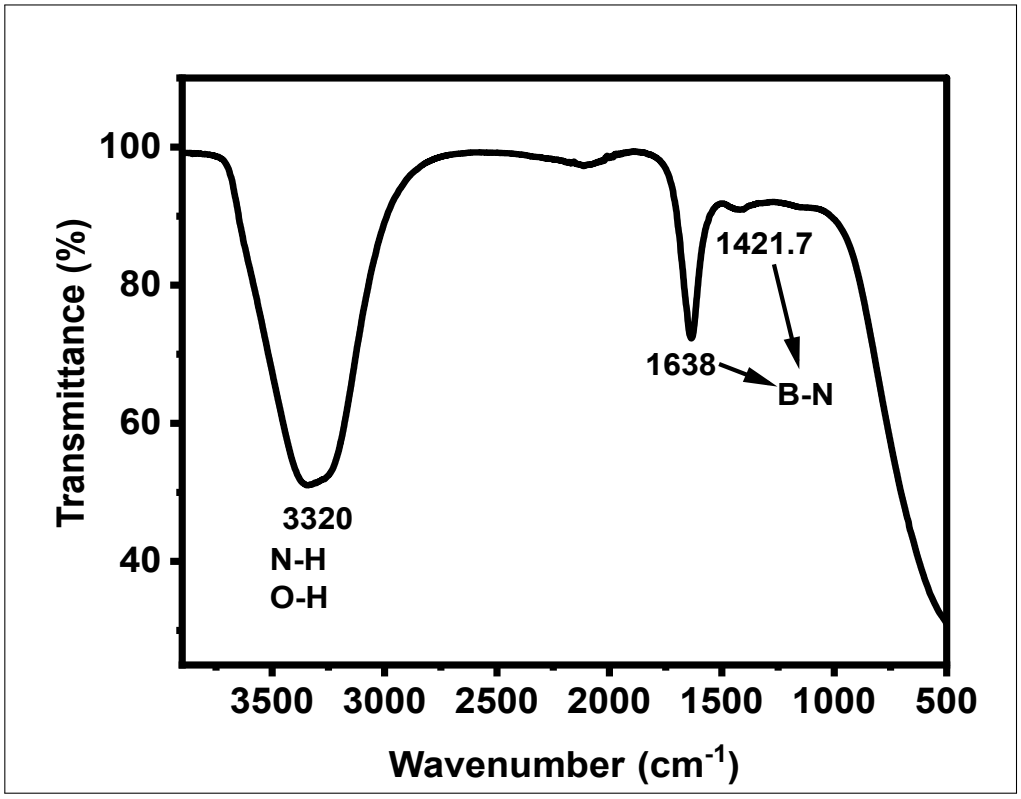

Figure S1. FTIR spectra of Boron nitride quantum dots (BNQDs), where the band at 3320 cm^{-1} corresponds to N-H, O-H stretching modes and at 1638 cm^{-1} and 1421.7 cm^{-1} corresponds to B-N stretching vibration.

Tauc plots representing the energy band gaps of S1 (a), S2 (b), S3 (c)

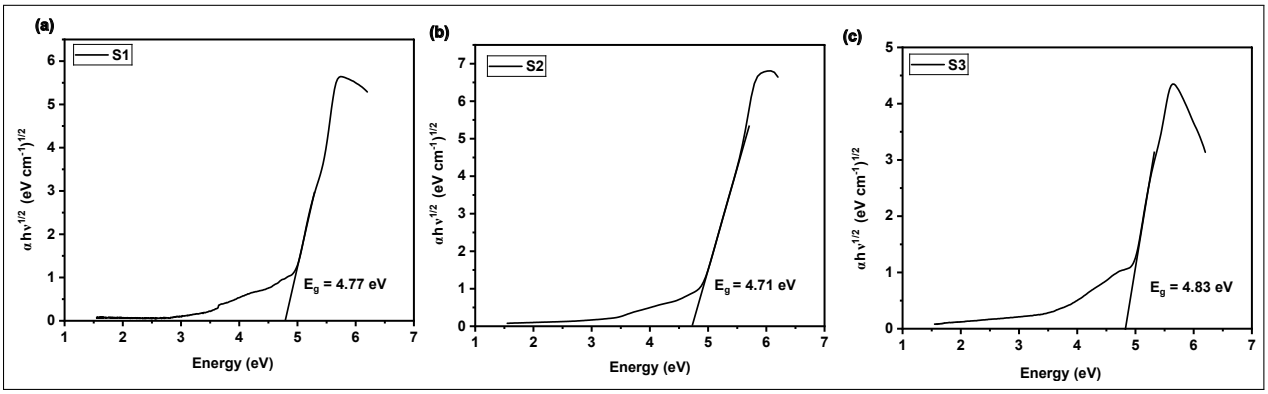

Figure S2. Tauc plots representing the energy band gaps of S1 (a), S2 (b), S3 (c)

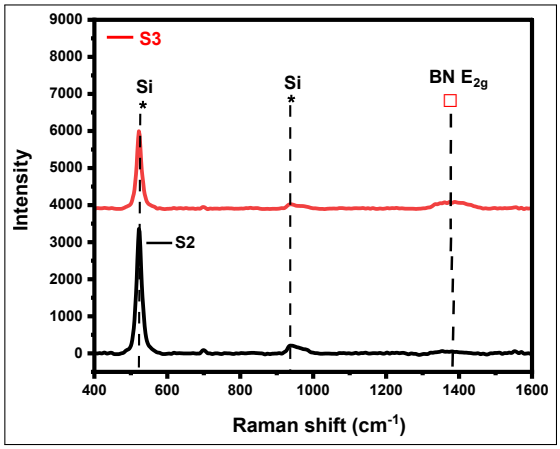

Figure S3. Raman spectra of S2 and S3 on Si substrate where, the peaks at 520 and 935 cm^{-1} corresponds to Silicon substrate.

Table S1. **Absorption, emission and stokes shift values at different filling volume percentage at 200 °C of temperature for 24 h.**

Sample	Absorption (eV)	Emission (eV)	Stokes shift (meV)
S1	4.27	3.41	860
S2	4.21	3.32	890
S3	4.73	3.37	1360

II. Raman mesurements

The raman spectra was obtained for BNQDs sample on silicon substrate by spin coating. The BNQDs of 1.2 mg were dispersed in 1ml of ethanol. The spin coating was done in two steps, step 1 with 2000 rpm, and 30 s of time. Then, in step 2 the rpm of 5000, and time of 60 s were used. At each step 50 μl of BNQDs (1.2 mg/ml in ethanol) was used.

Electrochemical Characterization

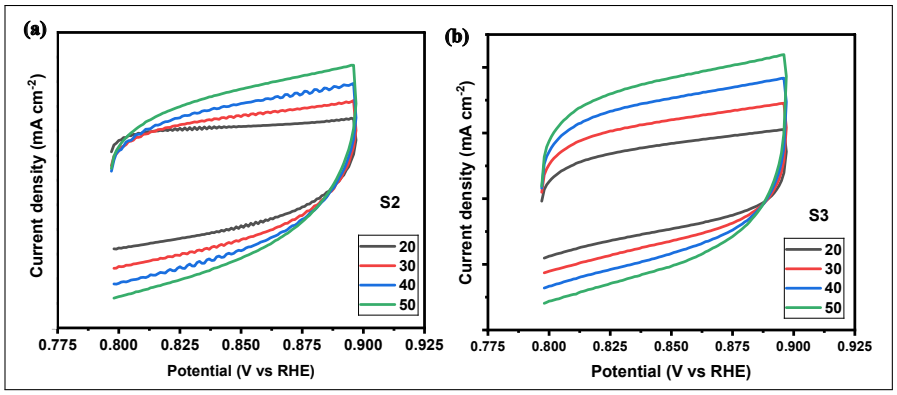

Figure S4. Double layer capacitance measurement at different scan rates from 20 mV/s to 50 mV/s of (a) S2 and (b) S3.

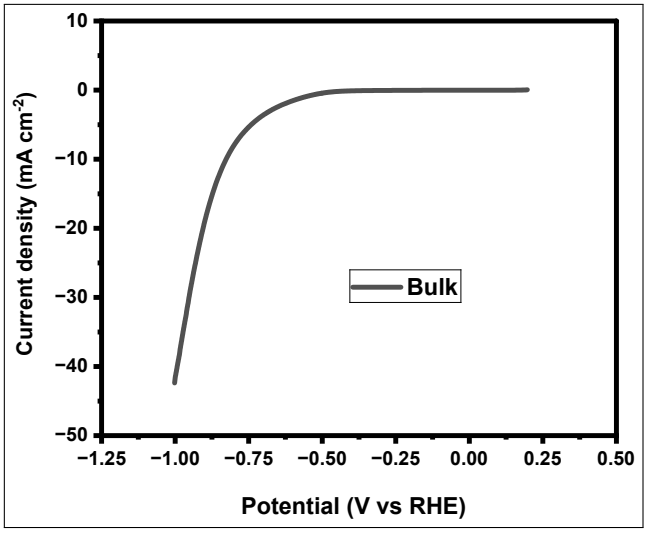

Figure S5. Linear sweep voltammetry of commercial bulk h-BN of 1μm size at scan rate of 50 mV/s in 0.5 M of H_2SO_4.

III. References

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