Electronic Supplementary Information for:

Controlled synthesis of monodispersed ZnSe microspheres for enhanced photo-catalytic application and its corroboration using density functional theory

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Figure S1

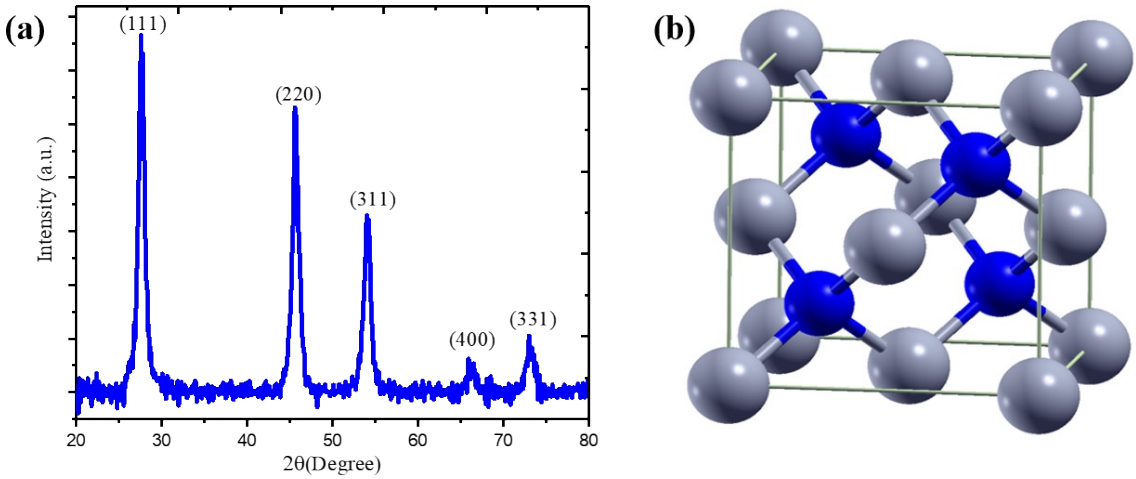

Figure S1: (a) XRD spectrum of EDTA optimized material (EDTA: 10 mmol, hydrazine hydrate: 15 ml, temperature: 180 °C, time: 2 hours) (b) Optimized crystal structure of bulk ZnSe. The grey spheres indicate Zn atoms, whereas the blue spheres indicate Se atoms.

The typical ZnSe material synthesized under experimental conditions as EDTA: 10 mmol, hydrazine hydrate: 15 ml, temperature: 180°C, time: 2 hours is subjected to structural analysis by XRD. The typical XRD pattern obtained is shown in figure S1. The XRD pattern is in good agreement with the standard JCPDS card no. 01-080-0021 (a = 5.618, space group = F-43m, space group no. 216). In the pattern peaks corresponding to (111), (220), (311), (400), and (331) planes are obtained which can be indexed to cubic ZnSe. The value of lattice constant 'a' as calculated by using the formula $2d\sin\theta = \lambda$ is a = 5.62 Å. No impurity peaks are seen in XRD which indicates the high purity of the sample. Also, the sharp nature of peaks indicates that the product has high crystallinity. The crystallite size is calculated by using Scherrer's formula $D = 0.9\lambda/(\beta \cos\theta)$, where 'D' is the average diameter of the nanoparticles formed, 'λ' is the wavelength of the X-ray source used, 'θ' is the Bragg angle of the X-ray diffraction and 'β' is the full width in radians at the half maxima of X-ray diffraction peak. The average value of 'D' is found to be 10± 0.5 nm.

Figure S2

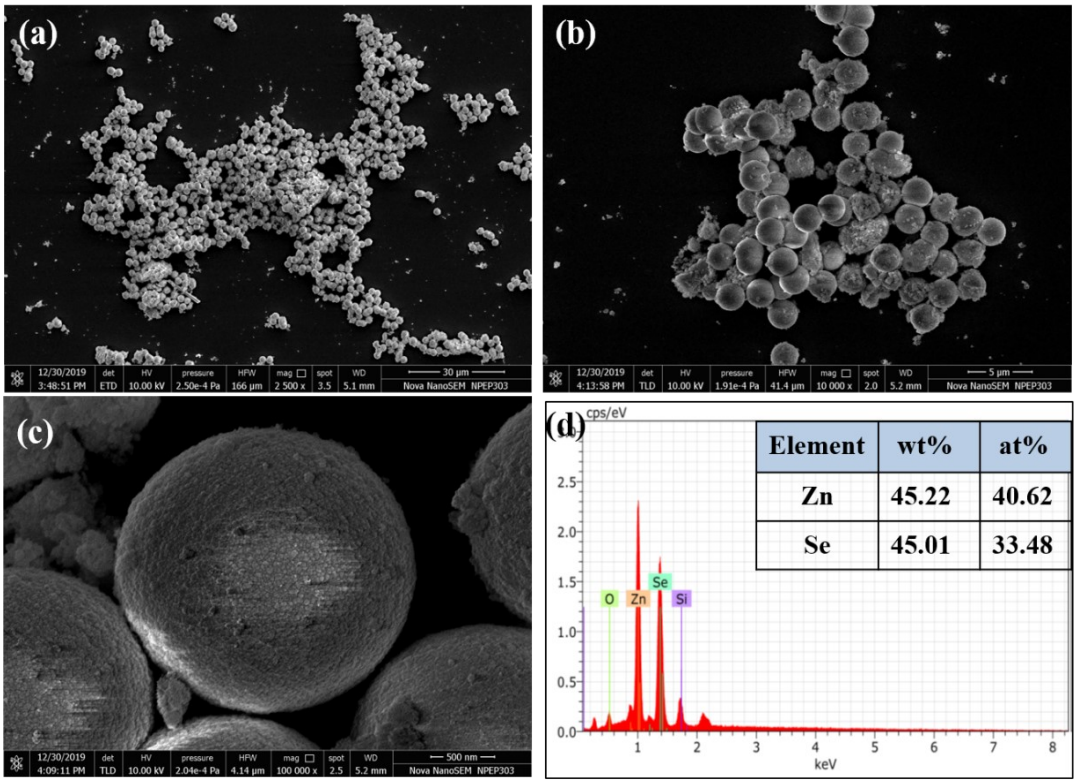

Figure S2: FESEM images of EDTA optimized material (EDTA:10mmol). (a), (b), (c) are FESEM images of material with different magnifications (d) EDS spectrum of the material synthesized by using 0 mmol of EDTA, 15 ml of hydrazine hydrate and maintained at 180 °C for 2 h.

Figure S3

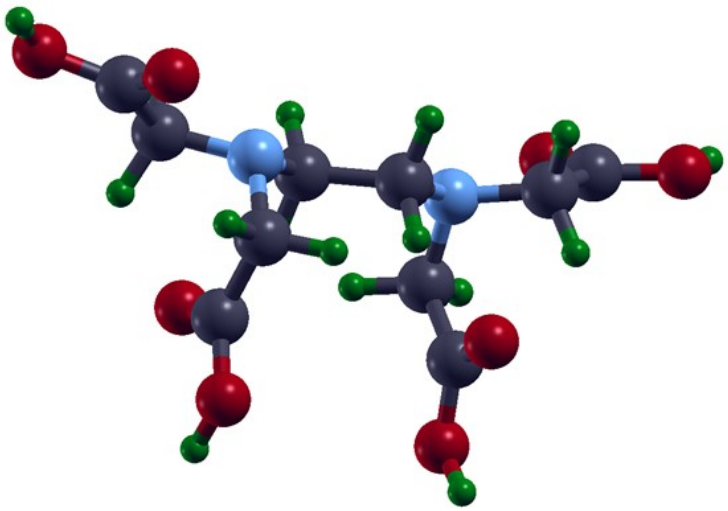

Figure S3: 3D structure of EDTA molecule. The red, grey, blue and green spheres represent respectively oxygen, carbon, nitrogen and hydrogen atoms.

Figure S4

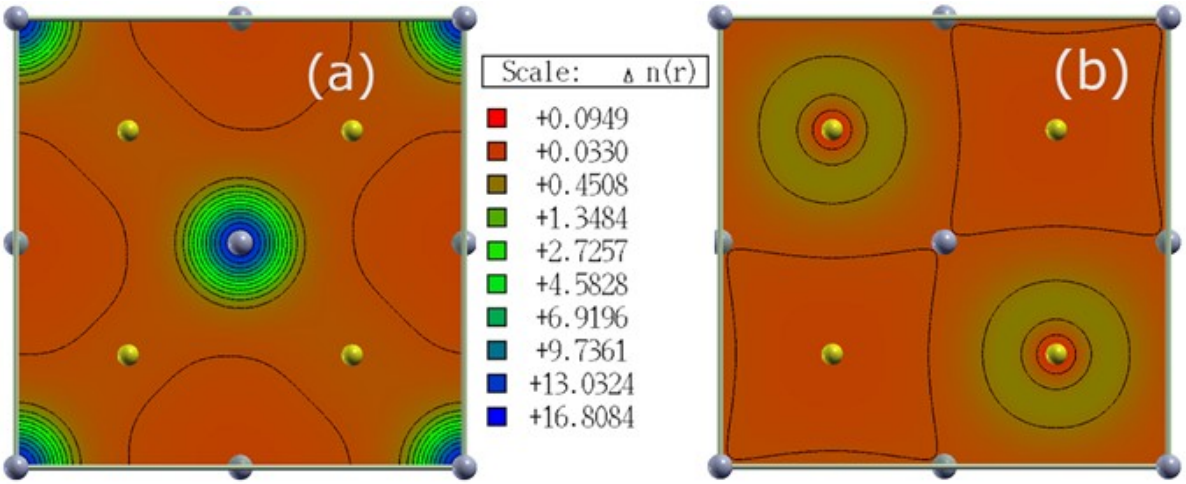

Figure S4: The electron density contours sliced in ZnSe (100) plane through (a) Zn atoms and (b) Se atoms plotted at $(1/10)^{th}$ of the maximum electron density value.

Figure S5

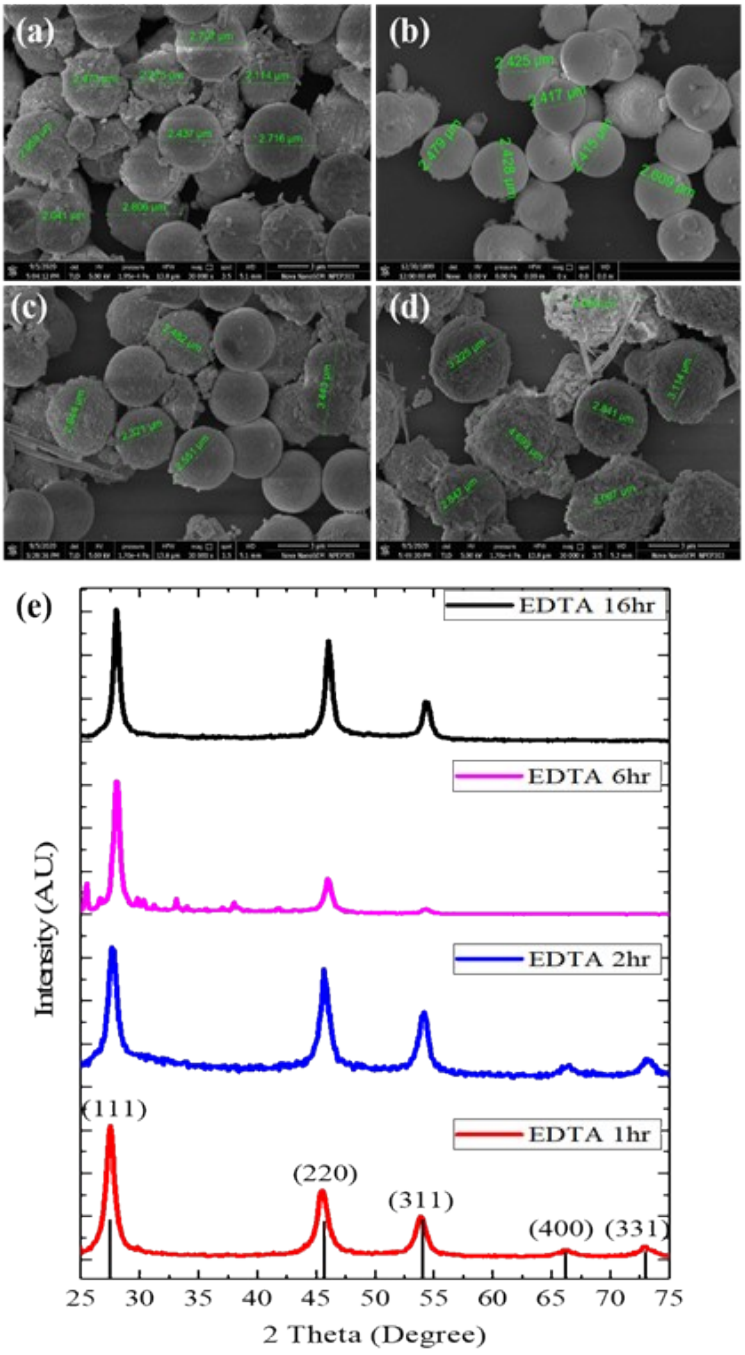

Figure S5: FESEM images of samples synthesized with different reaction times (a) 1 hr (b) 2 hr (c) 6 hr (d) 16 hr. (e) The XRD patterns obtained for samples with different reaction times.

Figure S6

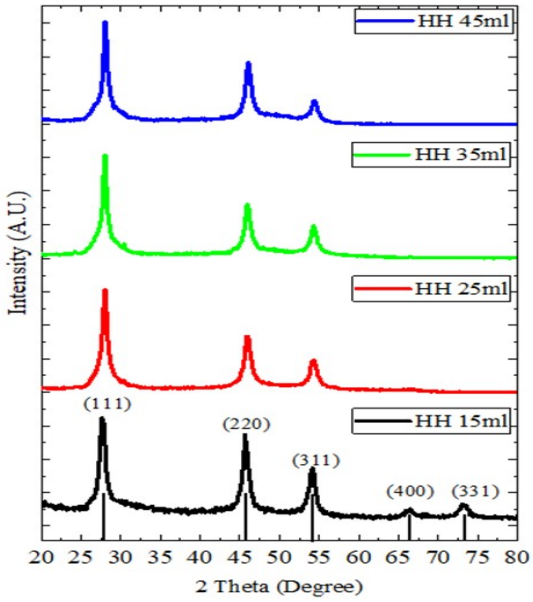

Figure S6: The XRD patterns of materials synthesized with different volume percentage of hydrazine hydrate.

Figure S7

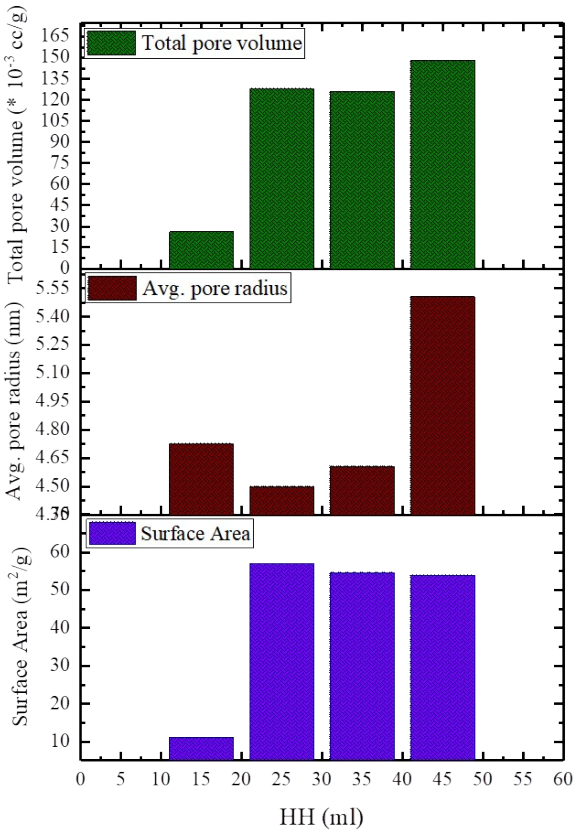

Figure S7: Variation of surface area, average pore radius and total pore volume with change in HH volume percentage.