

## **Supplementary Information**

### **Controlled Synthesis and DFT Insights Investigation of Novel 0(D)-(3D) ZnS/SiO<sub>2</sub> Heterostructure for Photocatalytic Applications**

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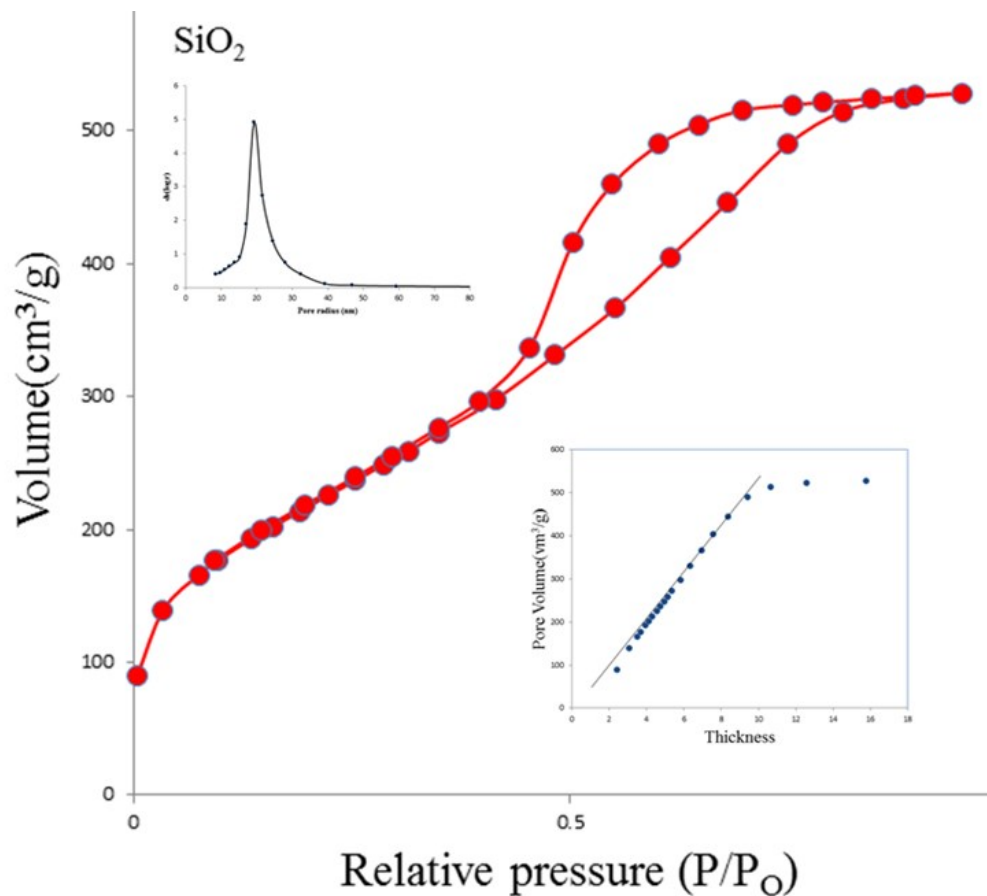
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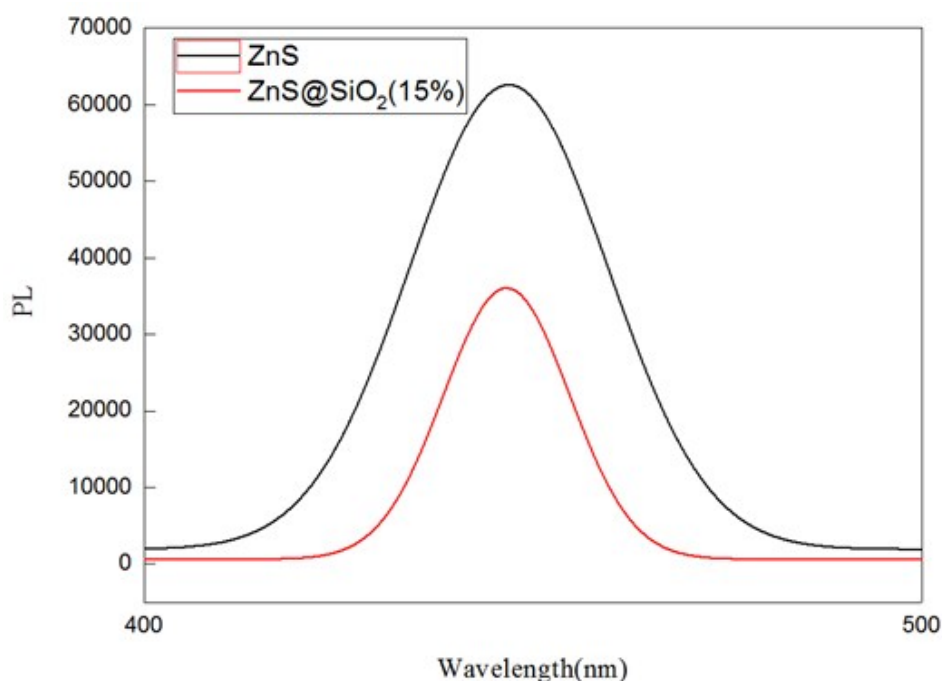
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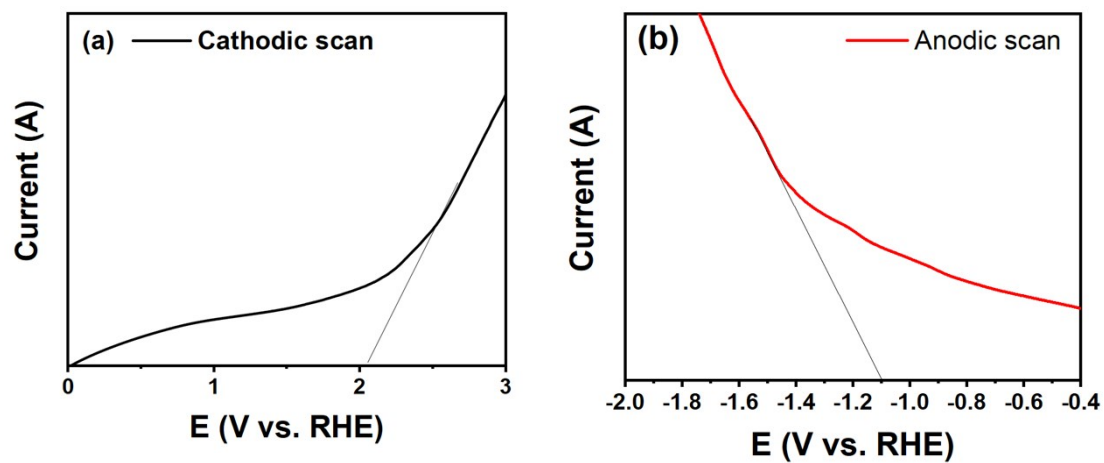


**Figure S1:** N<sub>2</sub>-adsorption-desorption isotherm, V-t (thickness) plot and pore size distribution and survey for SiO<sub>2</sub>. Results dedicates high surface area silica with type 4 isotherm with high surface area close to 800 m<sup>2</sup>/g.



**Figure S2:** Photoluminescence (PL) spectra of ZnS and ZnS/SiO<sub>2</sub> (15%).

PL reflects the defect appeared in the material lattice. Usually there is a competition between separation and re-combination of electron-hole pairs. In addition, the photo-degradation process is generally improved through the higher separation between electron and hole to increase its lifetime in the oxidation of organic pollutant materials. According to the Figure, the presence of a prevailing peak at 440 nm can be observed intensively, which come from the different defects in the ZnS crystalline structure. After incorporation of ZnS in silica gel matrix, a remarkable quenching of the ZnS peak can be observed reflecting the strong interaction among silica and zinc sulfide material.



**Figure S3:** Anodic and cathodic LSV scan of ZnS/SiO<sub>2</sub> (15%).