Towards visible light activity of wide band gap photocatalysts: Surface functionalization of ZnO with ZnS

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— We show that at the ZnO/ZnS interface the band alignment is favorable for reducing the photo excitation threshold energy; signifying that the combination of two wide band gap photocatalysts can yield a material with visible light activity. Modification of ZnO with a sub monolayer ZnS is investigated by scanning tunneling microscopy (STM) and photoemission spectroscopy. STM studies indicate that the ZnS grows by nucleation and spreading of 2D clusters of monolayer height (\(\sim 2.5 \, \text{Å}\)). Photoemission spectroscopy is used to measure the band alignment between ZnO and ZnS, as well as measure the changes in the surface charge region and work function. An increase in work function by 1.1 eV is observed and a staggered band alignment is found with ZnS states effectively narrowing the band gap for photo excitation from 3.4 to 2.7 eV. We propose that the combination of these structural and electronic properties of the modified ZnO surface result in an improved, visible light active photocatalyst.

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