Electroluminescence in Zinc Sulfide and Doped Zinc Sulfide Materials

Investigations of Electroluminescence of Zinc Sulfide and Doped Zinc Sulfide Materials Synthesized in Microgravity

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In Short

- Evaluation of the electronic structures of ZnS and doped ZnS materials
- Optimized hybrid functionals for ZnS and ZnS doped materials
- Defect calculations for ZnS and ZnS doped materials
- Develop the explanation for the fundamental phenomena of electroluminescence in our synthesized materials

The work herein aims at improving the energy efficiency of electroluminescent zinc sulfide (ZnS) doped materials that were synthesized in microgravity. Screens and displays consume tremendous amounts of power. Global trends to significantly consume less power and increase battery life have led to the reinvestigation of electroluminescent materials for usage in screens and displays. The state of the art in ZnS materials has not been furthered in the past 30 years and there is much potential in improving electroluminescent properties of these materials with advanced processing techniques and numerical analysis [1].

These new advanced zinc sulfide doped materials are synthesized with a new process involving a rapid exothermic process involving high energy and nonlinearity coupled with a high cooling rate to produce materials formed outside of normal equilibrium boundaries (under patent). The elimination of gravity driven buoyancy results in a superior and enhanced homogeneity in the synthesized materials. ZnS and ZnS doped materials are synthesized at the Center of Applied Space Technology and Microgravity (Zentrum für angewandte Raumfahrttechnologie und Mikrogravitation, ZARM) drop tower. Utilizing this process with ZnS doped with elements such as Cu, Mn, Eu, Pr leads to electroluminescence (EL).

Unfortunately, characterization of these synthesized materials alone are insufficient in the identification of specific defects and explanation of electroluminescence in semiconductor materials. It is necessary to perform theoretical calculations parallel with characterization of our synthesized materials to identify intrinsic and extrinsic defects.

It is planned in this work to optimize hybrid functionals (HSE-type) for different phases of ZnS and doped ZnS, study the defects, and then examine the charge transition levels and hyperfine interaction of these structures. The HSE parameters will be refined, thus allowing a more exact comparison when using existing models with our above findings and explain electroluminescence in our materials. It is only with this understanding in the underlying phenomena as to how light is produced in ZnS doped materials that we can truly increase the efficiency of these promising materials.

The first major shortcoming of zinc sulfide doped electroluminescent materials is that there is currently no numerical relation between particle size, crystal structures, combinations of structures and phases, stoichiometry, nonstoichiometry, strain, dislocations, vacancies, interstitials, dopants, intrinsic and extrinsic properties, recombination effects, and energy transfer to electroluminescence. It is well known that this material can emit light and there are general theories of luminescence, but there is no solid relationship between this and the materials properties listed above. A.H. Kitai and Surjit S. Chadha et al. have summarized the general theories of EL and the relations to powder EL, but this is only a summary of the production and measurements of these powders [2].

The second shortcoming of zinc sulfide doped materials is there no exact explanation for the fundamental phenomena of electroluminescence in this material on any level including power to thin films. Electroluminescence is a phenomenon that does not consist of only one single process [3]. Different processes may occur depending on the localized energy levels of the material and the local conditions of the electric field. To briefly describe electroluminescence, the energy from the electric field is used to excite the material into a more energetic state by the generation of free charge carriers (excitation). Next, the free carriers move through the material (transport). Third, oppositely charged carriers recombine (recombination). It is viewed that only the radiative recombination is of importance for electroluminescence and the transportation process might be negligible. The extensive evaluation from the last 60 years yielded insight to two predominate excita-

tion processes. These processes are impact ionization/excitation and minority-carrier injection where Piper et Al. and Maeda et al. presented promising approaches [4-5]. These will be evaluated with respect to the structural properties listed above.

The work proposed above includes the examinations of the optimization of the HSE-type hybrid functionals for ZnS and doped ZnS, defect calculations, hyperfine interactions, and the photoluminescence of dopants.

We have begun this work with the optimization of the HSE-type Hybrid Functional for ZnS.

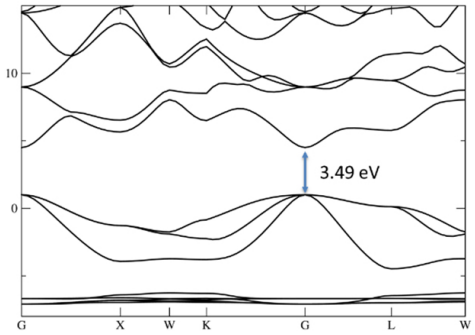

Figure 1: *The electronic structure of zinc sulfide (Sphalerite, FCC) illustrating 3.49 eV for the band gap at the first significant point (K point) in the Brillouin zone.*

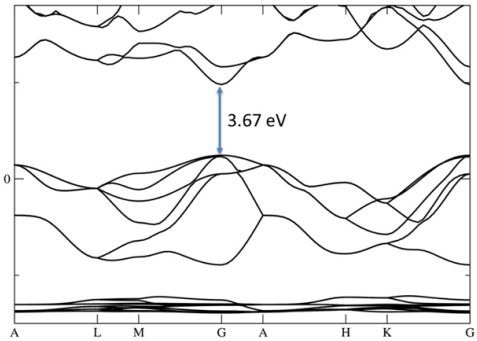

Figure 2: *The electronic structure of zinc sulfide (wurtzite structure, hexagonal) illustrating 3.67 eV for the band gap at the first significant point (K point) in the Brillouin zone.*

First, the electronic structure of zinc sulfide for sphalerite (FCC) and wurtzite structure (hexagonal) was calculated and is shown above in Figures 1 and 2 respectively. This analysis utilized a small unit cell (2 atoms) whereby the band gaps were calculated for the first significant point in the Brillouin zone (K point). This calculation utilized density functional theory (DFT) with hybrid exchange within the Vienna Ab initio Simulation Package (VASP) package. DFT underestimates the band gaps of semiconductors, due to an error estimation calculation. Measured band gaps of the zinc blend material were measured 3.70 eV and this has excellent correlation with our calculated value of 3.49 eV [6]. Furthermore, measured band gaps of the wurtzite structure were measured at 3.77 eV and this has excellent correlation with our calculated value of 3.67 eV [7]. The results here were calculated with non-optimized parameters HSE (0.30,0.20). These will be refined in the future.

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More Information

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Project Partners

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