Electroluminescence in Zinc Sulfide and Doped Zinc Sulfide Materials

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

***Q. D. Ho, M. Castillo, M. Thode**, The Center of Applied Space Technology and Microgravity (ZARM), University of Bremen*

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 general work herein aims at understanding and improving the energy efficiency of electroluminescent zinc sulfide (ZnS) doped materials there are 2 parts in our work. In the experimental part, ZnS and ZnS doped materials are synthesized at the Center of Applied Space Technology and Microgravity (Zentrum fÃ¼r angewandte Raumfahrttechnologie und Mikrogravitation, ZARM) drop tower. Unfortunately, characterization of these synthesized materials alone is insufficient in the identification of specific defects and in the explanation of electroluminescent origins in semiconductor materials. It is necessary to perform theoretical part parallel with the characterization of the synthesized materials in order to identify intrinsic and extrinsic defects. The operation of semiconductors-based devices is related to defects, which control electronic and optical behavior. The commonly used approximation, density functional theory (DFT) with LDA or GGA exchange, often fail completely in describing defects in wide band gap semiconductors. In recent years, screened hybrid functionals (like HSE06) have emerged as a useful alternative. This project will deal with the possible refinement, extension and application of the HSE-type functionals for defects in sphalerite and wurtzite ZnS. We will study charge transition levels, hyperfine interaction, and luminescent origins in ZnS at the aims of improving electroluminescent ZnS-based devices.

It is well known that ZnS can be a very potential material that can be used as display panel at extreme conditions, but there are no solid justifications of luminescent origins in this semiconductor material. The functionality of semiconductor devices is strongly connected to defects that determine electric and optical behavior of the semiconductor. For using ZnS-based luminescent devices it is necessary to fully understand and identify defects in ZnS. However, there are several challenges for defects theory. Defects calculations require two things: a suitable model for the system and an appropriate model. With the development of computer, it is easy to get a good model size for the calculation that we will discuss later in section 1.4.1 for the approximation. Density functional theory is the commonly used model for semiconductors. However, DFT with semi(local) exchange, has failed completely with wide band gap semiconductors. The failure of traditional DFT exchange approximations is related to the lack derivative discontinuity at integer occupation numbers and convex behavior of total energies as a function of the fractional occupation numbers instead of being linear. These problems cause semiconductors band gap underestimation and artificial delocalization of defects states. Consequently, the actual defects can be hidden in the bands, incorrect occupies resulting hyperfine interaction can be found correctly. Recently, (semi)local DFT and GW [1] methods are often applied for electronic structure determination, but their defects calculations have problems and total energy methods (like RPA) cannot be applied to supercells which are required for determination defects in semiconductors [2]. Therefore, we are going to use hybrid functionals, which are emerge recently as a useful alternative, for defects studies in ZnS.

The hybrid functional HSE06 (0.25,0.20) are generally used in semiconductor calculations and yields the best results of band gap for many semiconductors. However, the value chosen in HSE06 works well only with a medium-size gap (and medium screening). However, when the standard HSE06 underestimates the band gap, only α is often tuned and the role of the screening parameter is neglected. In doing so, the issue of the localization of defect states is not usually considered even though it has been shown that accurate description of small polaron states can only be expected if the generalize Koopmansâ theorem (gKT) is satisfied [3] i.e., if the total energy is a linear function of the fractional occupation numbers. Non local and semi(local) exchange has opposite behaviors of total energies as functions

of occupation numbers. Thus, HSE-type hybrids give an opportunity to mimic the exact exchange by error compensation, but as discussed above both of α and μ should be tuned parallelly, to obtain the total energy as a piecewise linear function of the occupation numbers and the total band structure should agree to GW calculations. We call the hybrid functional-types that meet those two criteria is optimized hybrid functional. The success of using the optimized hybrid functionals has been shown with $CuGaS_2$, CuGaSe, CuInS, and β-Ga_2O_3 [4-7]. The calculated band gap, defects charge transition levels hyperfine interaction and luminescent radiation from the optimized can be compared directly and agree very well to the experimental results [4-6,8].

Another shortcoming of zinc sulfide doped material display application is that there is 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, different processes may occur and many defects can be involved or used to explain origins of luminescent centers [5]. Therefore, in our research we will study both of intrinsic, extrinsic and complex defects to pin the Fermi-level and explain the origins of luminescence. This effort will be very time and resources consuming.

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More Information

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