# Fundamental understanding of electronic and optical properties of the synthesized $Sb_2S_3$ material and possible application

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Since antimony sulfide´s ($Sb_2S_3$) could be a promising candidate in solar energy conversion industry (as an absorbing material), we concentrate on the detailed experimental and theoretical investigations of the structural, and generally poorly investigated electronic and optical properties of this synthesized material with desired electronic properties. Concerning the applications of this material in the area of photovoltaic devices, certainly one of the most important parameters is the band gap energy that determines what portion of the solar spectrum a photovoltaic cell will absorb. The main characteristic of the calculated electronic structure is the significant improvement of the band gap value. The values of experimental band gap energies, found for the synthesized $Sb_2S_3$ nanowires *separated* in the form of bundles and *coalesced* with each other in long bars, are lower than theoretical ones for approximately 0.3 eV. We explained those differences firstly by temperature differences, since the difference in the band gap energy at 300 K (at which experiments were performed) and at 0 K (which theory gives), for different semiconductors can vary between 0.10 and 0.22 eV. Unfortunately, there are no data concerning band gap energy difference (for different temperature) for the semiconductor $Sb_2S_3$. Additional difference (assuming that the temperature difference makes a difference in energy of ~ 0.2 eV) of approximately 0.1 eV in the present work, can be explained by excitonic effects that cannot be neglected here due to the high calculated energy of an exciton. The excitonic effects calculated

are important in understanding physical effects of the usage of $Sb_2S_3$ in solar cells and fundamental understanding of this semiconductor that missing so far in the literature. Obtained high dialectric constant ($\varepsilon \approx 11$), and in the same time high energy of exciton (probably Wannier-Mott excitons) ($E_{ex} \approx 0.1$ eV and radius of exciton $a_x \approx 0.9$ nm ($m_e^* = 1.035m_e$ and $m_h^* = 1.843m_e$,)) make this semiconductor quite unique in comparison to other semiconductors used to date in solar cells, excitonic solar cells - Frenkel excitons. More detail analysis showed that there are arguments for the both basic types of excitons.

| Crystal | Eg (eV) | $R_X$ (meV) | $a_x$ (nm) |
|---|---|---|---|
| GaN | 3.5 | 23 | 3.1 |
| ZnSe | 2.8 | 20 | 4.5 |
| CdS | 2.6 | 28 | 2.7 |
| ZnTe | 2.4 | 13 | 5.5 |
| CdSe | 1.8 | 15 | 5.4 |
| CdTe | 1.6 | 12 | 6.7 |
| GaAs | 1.5 | 4.2 | 13 |
| InP | 1.4 | 4.8 | 12 |
| GaSb | 0.8 | 2.0 | 23 |
| InSb | 0.2 | (0.4) | (100) |
| $Sb_2S_3$ | 1.3-1.5 | 74 | 0.8-0.9 |

**Table 1.** The band gap ($E_g$) and calculated Rydberg constant ($R_x$) and Bohr radius ($a_x$) of the free excitons in several direct gap III-V and II-VI compound semiconductors. Values for the synthesized $Sb_2S_3$ semiconductor are obtained by 'integration' of the theoretical and the experimental results.

| Crystal | $m_e^*/m_e$ | $m_h^*/m_e$ |
|---|---|---|
| GaN | 0.13 | 0.8 |
| ZnSe | 0.13 | 0.65 |
| CdS | 0.19 | 0.8 |
| ZnTe | 0.12 | 0.5 |
| CdSe | 0.06 | 0.62 |
| CdTe | 0.05 | 0.46 |
| GaAs | 0.07 | 0.2 |
| InP | 0.08 | 0.3 |
| GaSb | 0.04 | 0.1 |
| InSb | 0.01 | 0.25 |
| $Sb_2S_3$ | 1.035 | 1.843 |

**Table 2.** The electron effective mass ($m_e^*$) and hole effective mass ($m_h^*$) for III-V and II-VI compound semiconductors. Values of the effective masses are obtained by 'integration' of the theoretical and the experimental results.

The semiconductor $Sb_2S_3$ surely could found better application, if we truly understand the electronic properties, such as band gap and energy of excitons, as important parameters for all processes concerning the solar energy device efficiency. In the same purpose, so in order to better understand $Sb_2S_3$ semiconductor we made a new $Sb_2S_3$/dye based working solar cell.