Understanding of point defect mechanism boosts photovoltaic performance of antimony selenosulfide

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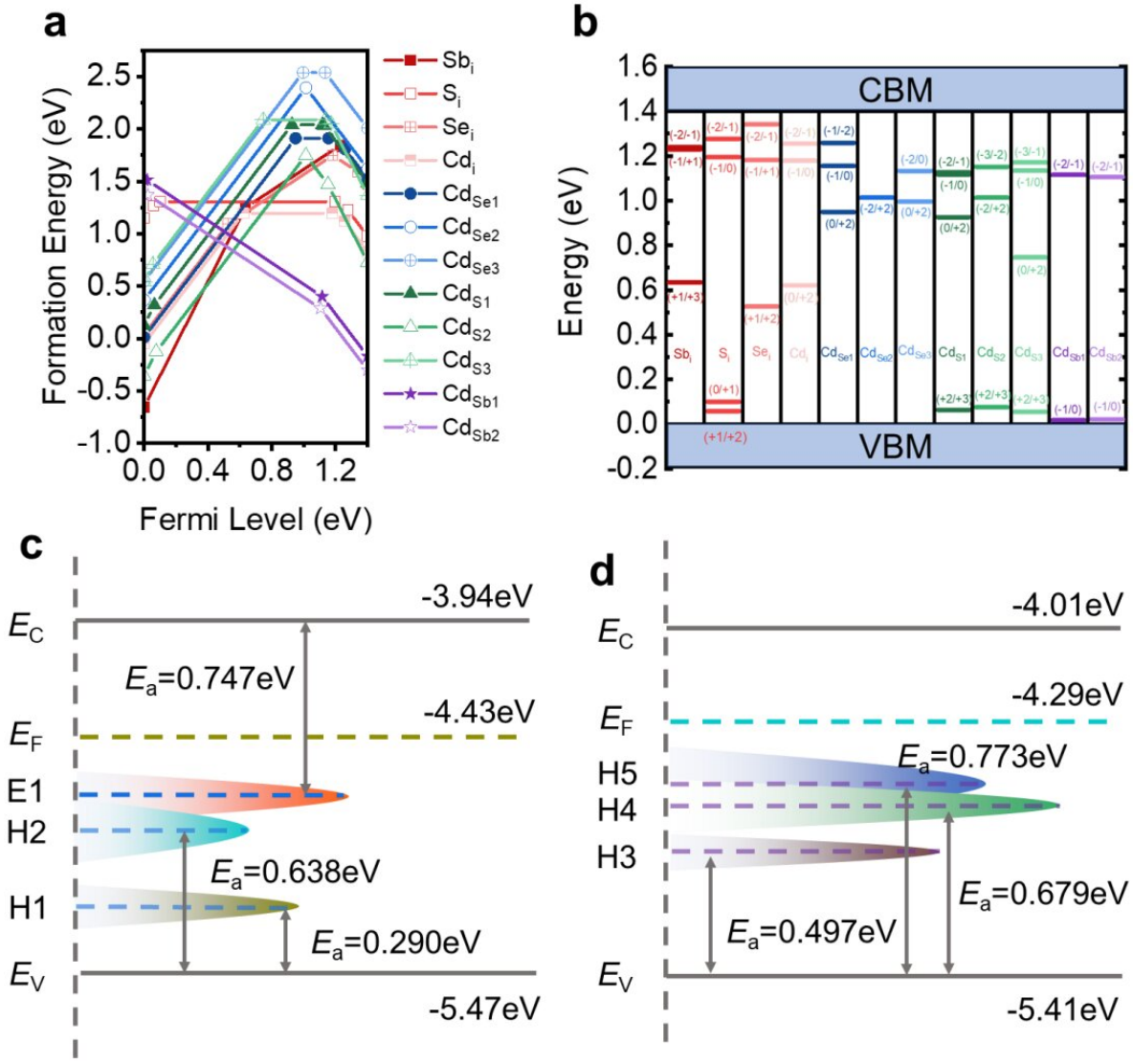

(a) Formation energy-Fermi level curves of interstitial defects in $Sb_2(S, Se)_3$ and the possible impurity defects caused by Cd doping. (b) Transition energy level diagram of defects. Defects energy levels of unannealed (c) and annealing at 350 °C (d) films. Credit: *Advanced Materials* (2022). DOI: 10.1002/adma.202208564

Recently, a research team led by Prof. Chen Tao from the University of Science and Technology of China (USTC) of the Chinese Academy of Sciences (CAS) revealed the formation and evolution of the point defect of antimony selenosulfide. This work was published in *Advanced Materials*.

Antimony selenosulfide, i.e., $Sb_2(S,Se)_3$, features great stability, no inclusion of rare or toxic elements, excellent photovoltaic property, and low cost, which make it an ideal photovoltaic material. Due to the quasi-one-dimensional structure and high extinction coefficient of the material, it has unique advantages in fields such as ultralight devices, portable power sources, or building-integrated photovoltaics.

To improve the performance of devices, it is necessary to understand the basic properties of this new photovoltaic material.. The research team focused on the point defect of antimony selenosulfide. They utilized optical deep-level transient spectroscopy (O-DLTS) to detect the characteristics of the defect of antimony selenosulfide driven by temperature. Researchers then investigated the variation of the material composition during annealing to reveal the formation and evolution of the point defect.

The initial hydrothermal deposition results in the formation of point defects with high formation energy, which was the result of random deposition of ions driven in hydrothermal condition, according to the

researchers. Post-annealing and the thin-film crystallization led to the loss of sulfur and selenium anions as well as the formation vacancy defect ($V_{S(e)}$). Since the formation energy of cation/anion inversion defects is relatively low, antimony ions would transfer and fill anion vacancies, eventually forming the $Sb_{S(e)}$ inversion defect.

The study deepens the understanding of the formation and evolution of point defects of antimony selenosulfide and offers a new method to study such processes. It also provides a guidance for designing methods to produce films and inhibiting the formation of deep-level point defects.

More information: Bo Che et al, Thermally Driven Point Defect Transformation in Antimony Selenosulfide Photovoltaic Materials, *Advanced Materials* (2022). DOI: 10.1002/adma.202208564

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