Inverse Design of High-Absorption Thin-Film Photovoltaic Materials

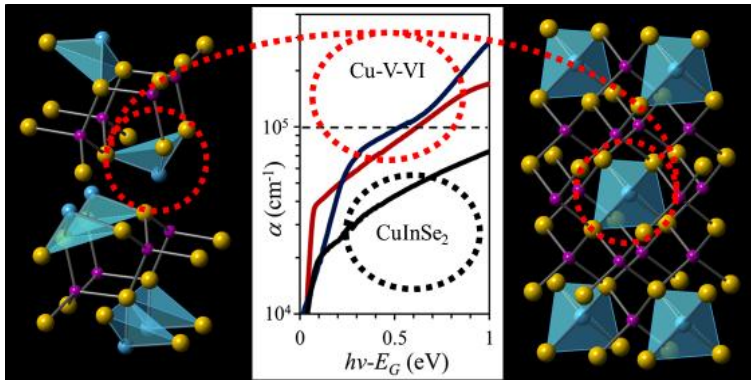
Scientific Achievement

Center for Inverse Design scientists identified some potential Cu-V-VI thin-film photovoltaic (PV) absorber materials that have stronger solar absorption than $CuInSe_2$—one of the most-studied thin-film PV absorber materials—and revealed a general structure–property (absorption) relationship.

Significance and Impact

The strongly absorbing materials that were identified can be incorporated into solar cells in very thin films. Also, they avoid using a low-Earth-abundant element such as In ($In/Si=10^{-7}$), thus offering a route to potentially scale thin-film PV to the terawatt level.

Research Details



Theory and experiment both indicate that some Cu-V-VI ternary materials, such as $CuSbS_2$ (left) and Cu_3SbS_4 (right), exhibit stronger solar absorption than $CuInSe_2$.

L. Yu, R. Kokenyesi, D. Keszler, and A. Zunger, *Advanced Energy Materials*, (2012) DOI: 10.1002/aenm.201200538

- The rapid onset to high absorption above the bandgap in Cu-M-VI (M = Group III-V) materials can be achieved by i) including M elements in low-valence states, or ii) Cu/M>1 cation stoichiometry.
- We used an inverse design approach:
  - i) The property of interest (here, solar absorption) was decided at the start.
  - ii) We applied the "spectroscopic limited maximum efficiency" metric, which reflects the target property to search for over a large space of compounds.
  - iii) Having found promising candidates, we selected a well-defined set of materials for detailed experimental and further theoretical examination. Thus, we avoided unconstrained studies of countless compounds.