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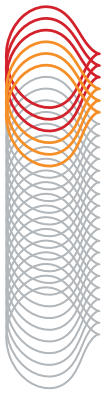
The Spectrum of Clean Energy Innovation



Fundamental Science

Market-Relevant Research

Systems Integration

Testing and Validation

Commercialization

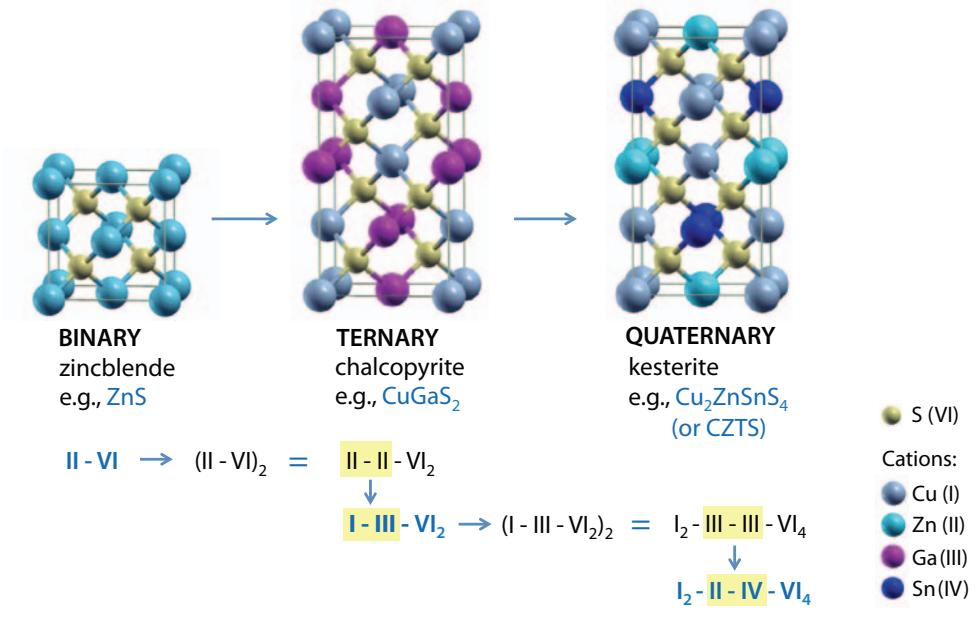
Deployment

NREL Explores Earth-Abundant Materials for Future Solar Cells

Researchers at the National Renewable Energy Laboratory (NREL) are using a theory-driven technique—sequential cation mutation—to understand the nature and limitations of promising solar cell materials that can replace today's technologies. Finding new materials that use Earth-abundant elements and are easily manufactured is important for large-scale solar electricity deployment.

The goal of the U.S. Department of Energy SunShot Initiative is to reduce the installed cost of solar energy systems by about 75% by the end of the decade. Obtaining that goal calls for photovoltaic (PV) technologies to improve in three main areas: solar-cell efficiencies, material processing costs, and scalability to the terawatt (TW), or 10^{12} watt, level. A promising route to simultaneously address all three SunShot challenges may be in discovering and evaluating novel, potentially efficient, and less costly Earth-abundant thin-film PV materials.

Sequential cation mutation is a systematic and theory-driven approach used to narrow a set of candidate materials that may be ideal for use in solar cells. By focusing on altering the composition one element at a time, researchers can examine changes in the optical, electrical, and structural properties of the material and determine which technologies can be further developed by experimentation to meet the SunShot Initiative's performance, cost, and scalability goals.



The evolution of crystal structures of binary, ternary, and quaternary compounds. To address concerns regarding indium and gallium scarcity, it has been proposed that CIGS can be replaced by $Cu_2ZnSn(S,Se)_4$ in the kesterite structure, in which every two group III (In or Ga) atoms in chalcopyrite structure are replaced by a Zn (group II) and Sn atom (group IV), a substitution that honors fundamental principles of chemistry.

Through deep technical expertise and an unmatched breadth of capabilities, NREL leads an integrated approach across the spectrum of renewable energy innovation. From scientific discovery to accelerating market deployment, NREL works in partnership with private industry to drive the transformation of our nation's energy systems.

This case study illustrates NREL's innovations in Fundamental Science through Market-Relevant Research.

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

Exploring the Promise of Quaternary Materials

In collaboration with researchers at Fudan University in China and University College London, researchers at NREL have performed systematic searches of quaternary semiconductors—compounds that consist of four elements, such as copper zinc tin sulfide (Cu_2ZnSnS_2, abbreviated as "CZTS") and related alloys. These materials can provide an Earth-abundant, thin-film alternative to today's choices, copper indium gallium diselenide (CIGSe) and cadmium telluride (CdTe). Using sequential cation mutation, researchers can derive and understand the material properties of the quaternary compounds by studying their evolution from binary (2-element) to ternary (3-element) compounds, and to quaternary compounds.

The quaternary CZTS semiconductor has drawn increasing attention recently as a strong candidate for a low-cost absorber material for thin-film solar cells that can be easily synthesized, with a high absorption coefficient ($>10^4$ cm^{-1}), which means it absorbs light well, and the optimal single-junction bandgap (~1.5 electron volts) for capturing sunlight and converting it to electricity.

CZTS is very similar to CIGSe in optical, electronic, and structural properties, as well as in methods of fabrication. Because of its similar thermal expansion and crystal lattice dimensions, CZTS benefits from CIGSe technology by using the same cadmium sulfide window layer and molybdenum back contact.

Unlike the ternary $CuInSe_2$ and binary CdTe-based solar cells, all the constituent elements in CZTS are naturally abundant and nontoxic. However, due to the complex nature of this quaternary compound, it has been unclear whether other quaternary compounds have physical properties applicable to solar cells. Through this research, the team has found that in addition to CZTS, the compounds $Cu_2ZnGeSe_4$ (CZGSe) and $Cu_2ZnSnSe_4$ (CZTSe) are also suitable quaternary materials for solar cell absorbers.

Assessing the Cell Structures of Candidate Materials

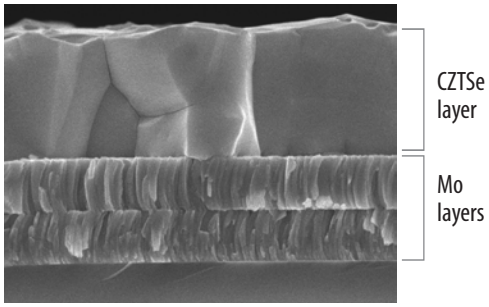
Chalcopyrite solar cells based on $CuInSe_2$, $CuGaSe_2$, and associated alloys have demonstrated high efficiencies, and production of these solar cells has increased as a result. However, the increased production has caused concern over manufacturing capacity because of possible indium and gallium scarcity. Consequently, kesterites, which are a related set of materials that comprise CZTS and associated alloys, have received increasing attention. Kesterite CZTS is similar to the chalcopyrite crystal structure, but with the indium and gallium atoms replaced in an ordered manner with an equal number of zinc and tin atoms. This maintains many of the optoelectronic properties of CIGS, but eliminates the need for the indium and gallium metals.

Currently, the record laboratory efficiency for a kesterite CZTS cell is 11.1%, as reported by IBM in 2012. This is about half that of CIGS cells. It is estimated that small-area solar-cell performance must exceed 20% to be a viable candidate for meeting the SunShot $0.50 per watt goal for modules and resulting in large-scale production.

To dramatically improve the performance of CZTS to meet the SunShot efficiency goals, NREL researchers are working to improve the fundamental understanding of the kesterite materials and apply this understanding to absorber processing, interface engineering, and device fabrication. Through the extensive study of defect and alloy properties of these materials, the researchers have confirmed that the growth of CZTS under Cu-poor/Zn-rich conditions to form a $Cu_2ZnSn(S,Se)_4$ alloy will be beneficial in improving the material properties, thereby maximizing solar cell performance.

NREL Experimentalists Make Progress in Developing Non-Toxic, Earth-Abundant CZTSe Solar Cells

Having shown the promise of CZT(S,Se)-based solar cells, NREL scientists are continuing to improve the conversion efficiency of CZTSe-based solar cells, which are one of the technologies based on non-toxic, Earth-abundant elements. NREL scientists have used commercially acceptable manufacturing techniques to advance the efficiency of CZTSe solar cells from zero to 8.4% in just 11 months, and recently reached 9.2% efficiency. The improvement is a result of focusing on defining the deposition process, which results in good composition control and morphology (as shown in the figure). NREL's next emphasis will be on controlling the surface properties and increasing the bandgap of the material to further increase the performance of CZT(S,Se) solar cells.



A scanning electron micrograph (SEM) image of a ~1.5-micrometer-thick polycrystalline CZTSe thin film. Growing films under Cu-rich conditions allows the growth of large crystals, which improves cell performance.

National Renewable Energy Laboratory

15013 Denver West Parkway
Golden, CO 80401
303-275-3000 • www.nrel.gov

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