Scientists Identify New Family of Iron-Based Absorber Materials for Solar Cells

Use of Earth-abundant materials in solar absorber films is critical for expanding the reach of photovoltaic (PV) technologies.

The use of Earth-abundant and inexpensive Fe in PV was proposed more than 25 years ago in the form of FeS_2 pyrite—*fool's gold*. Unfortunately, the material has been plagued by performance problems that to this day are both persistent and not well understood. Researchers from the National Renewable Energy Laboratory (NREL) and Oregon State University, working collaboratively in the Center for Inverse Design, an Energy Frontier Research Center, have uncovered several new insights into the problems of FeS_2. They have used these advances to propose and implement design rules that can be used to identify new Fe-containing materials that can circumvent the limitations of FeS_2 pyrite.

The team has identified that it is the unavoidable metallic secondary phases and surface defects coexisting near the FeS_2 thin-film surfaces and grain boundaries that limit its open-circuit voltage, rather than the S vacancies in the bulk, which has long been commonly assumed.

The materials Fe_2SiS_4 and Fe_2GeS_4 hold considerable promise as PV absorbers. The ternary Si compound is especially attractive, as it contains three of the more abundant low-cost elements available today. The band gap (E_g = 1.5 eV) from both theory and experiment is higher than those of c-Si and FeS_2, offering better absorption of the solar spectrum and potentially higher solar cell efficiencies. More importantly, these materials do not have metallic secondary phase problems as seen in FeS_2. High calculated formation energies of donor-type defects are consistent with p-type carriers in thin films and are prospects for high open-circuit voltages in cells.

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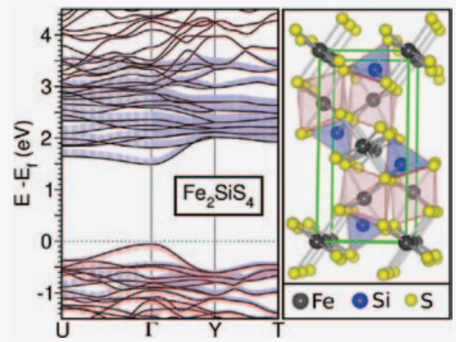
Reference: Yu, Liping.; Lany, S.; Kykyneshi, R.; Jieratum, V.; Ravichandran, R; Pelatt, B; Altschul, E.; Platt, H.; Wager, J.; Keszler, D.; Zunger, A. "Iron Chalcogenide Photovoltaic Absorbers." *Advanced Energy Materials* (2011) (accepted).



The electronic band structure (left) and the crystal structure (right) of Fe2SiS4. The Fe 3d bands (blue) give rise to desirable strong optical absorption.

Key Research Results

Achievement

Scientists have identified limitations of Fe-based absorber materials for solar cells.

Key Result

New insights into the long-standing low open-circuit problem of FeS_2 have been provided. A new family of Fe-based solar absorbers—based on the olivine member Fe_2SiS_4—has been identified. These materials offer a new entry point for the development of solar cells on the basis of stable materials containing Earth-abundant elements.

Potential Impact

Continued study and development of these materials could open new opportunities for introducing thin-film solar technologies that combine both low cost and high efficiency.

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