

Mechanism of long-used solar cell treatment explained by unexpected crystalline structure

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CdTe solar cells are the second-most common photovoltaic technology after silicon solar cells. In 2022, they represented about one-third of the U.S. utility-scale solar market. CdTe solar cells rely on a thin film of material to absorb light and convert it into electricity. Credit: Dennis Schroeder, NREL

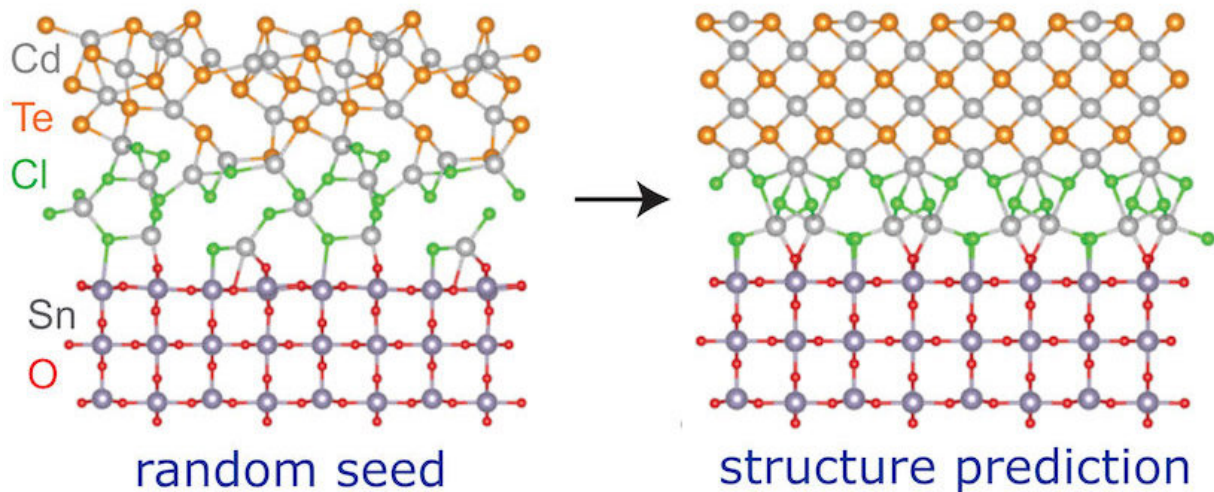
For more than three decades, photovoltaic researchers have known that the addition of a single chemical—cadmium chloride—creates better-performing cadmium telluride (CdTe) solar cells. But they have not understood exactly why, until now. The answer has implications for materials science that stretch well beyond solar cells.

The light-absorbing layers in CdTe [solar cells](#) are composed of a thin film of material, about 10–100 times thinner than a [human hair](#). Lots of modern devices, from solar [cells](#) to catalytic materials to organic light-emitting diode TVs, rely on thin-film materials. The surfaces at which these thin layers meet, or interfaces, are even thinner—100,000 times thinner than a human hair—and play a crucial role in the devices' functions. A better understanding of thin-film interfaces could improve how we fabricate many different materials, but the precise structure of interfaces at the [atomic scale](#) is often difficult to study.

A proven, but unexplained, boost for solar cells

In CdTe solar cells, the electrical charges created by an absorbed photon can be trapped and lost at the interfaces between the light-absorbing layer and the layers that carry those charges away into electrical circuits. As early as the 1980s, CdTe researchers realized that treating the interfaces in the solar cell with a small amount of cadmium chloride (CdCl_2) could reduce the loss of charges at the interfaces and improve the solar cell's power conversion efficiency.

Clearly, the addition of CdCl_2 changed the [interface](#) in a crucial way. But further experiments could not resolve the interface's structure down to the atomic level to explain why the CdCl_2 treatment was so effective. This challenge is not unique to CdTe solar cells. Interfaces are notoriously difficult to study and understand at the [atomic level](#), especially in cases of nonideal interfaces between materials that have different crystal structures.



The researchers determined the most stable arrangement of cadmium and chlorine atoms at the interface of tin oxide (SnO₂) and CdTe crystals through a structure prediction algorithm. The algorithm generated initial random arrangements of atoms at the interface (left), then updated those arrangements many times and allowed them to relax to their most stable arrangement (right). This revealed that CdCl₂ in the interface assumes a unique arrangement not found in larger crystals of the material. This interface-specific atomic structure explains how the CdCl₂ treatment improves the performance of CdTe solar cells. Credit: *Applied Physics Reviews* (2022). DOI: 10.1063/5.0104008

Modeling offers new insights into interfaces

A new approach from a team of National Renewable Energy Laboratory (NREL) researchers and colleagues at Khalifa University, Bowling Green State University, and First Solar—an American CdTe solar manufacturer—has unmasked the details of the CdCl₂ interface treatment. By modeling the behavior of individual atoms and electrons, the team simulated possible arrangements for CdCl₂-treated interfaces.

To calculate the electronic structure of a CdTe solar cell—and thereby

determine its charge collection—the researchers first needed to determine the atomic arrangement CdCl₂ interface, which had never before been done for CdTe solar cells. To achieve this, the team implemented a structure prediction algorithm for interfaces. The algorithm began with a random arrangement of atoms and then allowed them to settle, using a method called density functional theory to calculate the atomic forces. The algorithm repeatedly made small but realistic changes to the positions of the atoms at the interface, which allowed the team to identify the lowest-energy (most stable) structures.

The work is published in the journal *Applied Physics Reviews*.

More information: Abhishek Sharan et al, Atomically thin interlayer phase from first principles enables defect-free incommensurate SnO₂/CdTe interface, *Applied Physics Reviews* (2022). [DOI: 10.1063/5.0104008](https://doi.org/10.1063/5.0104008)

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