# SEMICONDUCTOR OPTIMIZATION



# FIRST SOLAR REDEFINES PHOTOVOLTAIC MATERIAL DEFECTS WITH HPC MODELING & SIMULATION

With more than 13.5 gigawatts sold worldwide, enough to power more than 2 million homes, First Solar is a globar leader in photovoltaic solar energy solutions. The performance of semiconductor devices such as solar cells depends strongly on the properties of materials used in their fabrication. Deep understanding of these properties and the ability to tune them is critical for the development of new generations of advanced photovoltaics and electronics. First Solar, the world's largest manufacturer of thin-film solar panels, is using AweSim resources from the Ohio Supercomputer Center (OSC), to predict and optimize semiconductor properties in crystalline structures such as cadmium telluride (CdTe). Although the efficiency of commercial CdTe photovoltaic material has grown dramatically in recent years, the advances in performance and

## VIRTUAL DESIGNS. REAL BENEFITS.

stability of CdTe devices are achieved mostly through costly experimentation and process development while lacking theoretical guidance.

Through First Solar's research and development, their large-scale solar farms can deliver energy to utilities at prices that are lower than fossil fuels.



*"Our research is aimed on theory-driven understanding and optimization of CdTe-based solar cells performance and stability for clean energy generation."* 

— Dmitry Krasikov, development engineer at First Solar







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#### THE CHALLENGE

Cadmium telluride (CdTe) semiconductor, used for decades in X-ray detectors, has recently become the material of choice for the multi-gigawatt-per-year, thinfilm photovoltaic industry. The semiconducting properties of CdTe is determined by the structures of pure crystals and imperfections, or defects. While the word "defects" often carries negative meaning, it is the defects in CdTe that make them useable in practical applications. Engineers can intentionally introduce defects to give semiconductors unique, application-specific properties. The concentrations of defects and their positioning in the device structure define the electrical behavior of the device, but these depend strongly on the process conditions, such as annealing temperatures, quenching rates and field operation conditions.

#### THE APPROACH

To understand and describe the processes that affect the defects of CdTe, engineers first need to know the fundamental parameters of defects and reactions. First Solar uses theoretical calculations of the parameters of defects and reactions, such as defect formation energy, reaction energy and energy barriers of elementary processes, to feed the models describing the formation and evolution of defect concentrations and recharge of the defects. These accurate, state-of the-art methods require considerable parallel computational resources to treat systems large enough within a reasonable time frame.

### THE SOLUTION

By using high performance computing to process these large data models, First Solar is able to continute innovating in advanced technologies that lower electric costs, increase energy yield and provide stable and reliable grid integration. Through First Solar's research and development, their large-scale solar farms can deliver energy to utilities at prices that are lower than fossil fuels.



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