High-Throughput Identification of Materials for Silicon Tandem Solar Cells

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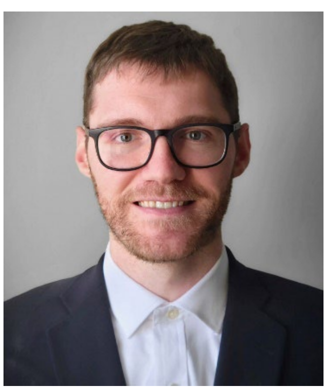
Abstract

Today, more than 90% of the market share of solar energy uses silicon (Si) as an absorber material. However, it is well established that Si is not an optimal light absorber as it has a band gap that is both indirect and lower than ideal according to the Shockley–Queisser efficiency limit. While some researchers seek alternate technologies to supplant silicon solar cells, building on the existing success of Si is the most efficient way to increase PV deployment. Therefore, a dual-junction device is desirable, which uses two materials to absorb different portions of the solar spectrum in the same cell rather than one in so-called "tandem" cells.

High-throughput calculations are employed to identify the most promising materials for silicon tandem solar cells. Starting with the Materials Project database of more than 131,000 materials, we evaluate the relevant properties of thermodynamic stability, lattice mismatch with silicon, band gap, effective mass, optical absorption coefficient and dynamic stability. The identified 11 optimal candidates represent a variety of material chemistries with oxides, pnictogenides, and chalcogenides included. Among them, perhaps the most promising is $Cu_2ZnSiSe_4$, which has almost ideal properties for all physical criteria and is composed of relatively earth-abundant constituents.

Short Biography



Lee A. Burton finished his PhD in 2014 at the University of Bath in the UK. Since then he has been awarded 2 international fellowships to undertake research in Japan and Belgium. For his work as part of The Materials Project, screening all known materials for various applications from catalysis to hydrogen storage, he was awarded the European Seal of Excellence in 2018.

After founding a group at Shanghai University in 2019, he is now beginning a new chapter as Senior Lecturer at Tel Aviv University; building on his expertise with big data to effectively incorporate machine learning into the process of property prediction and materials discovery.