The bulk photovoltaic effect in polar oxides for robust and efficient solar energy harvesting

Andrew M. Rappe

University of Pennsylvania

Solar energy is the most promising source of renewable, clean energy to replace the current reliance on fossil fuels. Ferroelectric (FE) materials have recently attracted increased attention as a candidate class of materials for use in photovoltaic devices. Their strong inversion symmetry breaking due to spontaneous polarization allows for excited carrier separation by the bulk of the material and voltages higher than the band gap (Eg), which may allow efficiencies beyond the Shockley-Queisser limit. Ferroelectric oxides are also robust and can be fabricated using low cost methods such as sol-gel thin film deposition and sputtering. Recent work has shown how a decrease in ferroelectric layer thickness and judicious engineering of domain structures and FE-electrode interfaces can dramatically increase the current harvested from FE absorber materials. Further improvements have been blocked by the wide band gaps (Eg =2.7-4 eV) of FE oxides, which allow the use of only 8-20% of the solar spectrum and drastically reduce the upper limit of photovoltaic efficiency.

In this talk, I will discuss new insight into the bulk photovoltaic effect, and materials design to enhance the photovoltaic efficiency. We calculate from first principles the current arising from the "shift current" mechanism, and demonstrate that it quantitatively explains the observed current. Then, we analyze the electronic features that lead to strong photovoltaic effects. Finally, we present new oxides that are strongly polar yet have band gaps in the visible range, offering prospects for greatly enhanced bulk photovoltaic effects.