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Visible light absorption in La, Cr co-doped $SrTiO_3$ and $BaTiO_3$ for ferroelectric photovoltaics RYAN COMES, MARTIN MCBRIARTY, PHUONG-VU ONG, Pacific Northwest National Lab, STEVE HEALD, Argonne National Lab, GERARD CARROLL, DANIEL GAMELIN, University of Washington, KEREN FREEDY, University of Virginia, SERGEY SMOLIN, JASON BAXTER, Drexel University, TIFFANY KASPAR, MARK BOWDEN, PETER SUSHKO, SCOTT CHAMBERS, Pacific Northwest National Lab — Ferroelectric materials offer intriguing possibilities as photovoltaic materials, as their built-in electric field is ideal for separation of optically-excited electron-hole pairs without the need for a p-n junction. However, the majority of ferroelectrics suffer from a wide optical band gap outside the visible range. By co-doping La and Cr into epitaxial $SrTiO_3$ and $BaTiO_3$ (SLTCO/BLTCO) thin films, we show that absorption in the visible light regime can be achieved with a band gap of ˜2.3 eV while preserving ideal stoichiometry. Through x-ray photoelectron spectroscopy, spectroscopic ellipsometry, photoconductivity and ultrafast pump-probe transient reflectance measurements, we show that visible light excitation of Cr 3d valence electrons into the Ti 3d conduction band produces optical carriers. Using piezoresponse force microscopy and polarized x-ray absorption fine structure measurements, we measure the ferroelectric polarization of the doped BLTCO films. These results are compared to density functional theory models to understand the optical and structural properties of the materials.

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