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Multigap Semiconducting ferroelectric perovskites LAI JIANG, ILYA GRINBERG, FENGGONG WANG, PETER DAVIES, ANDREW RAPPE, University of Pennsylvania — The energy conversion efficiency of a solar cell is directly related to the band gap of the material. By doping ferroelectric perovskites with Bi^{5+} on the B-site, we propose low band-gap materials suitable for bulk photovoltaic effect and related solar applications.Our DFT calculations indicate that the low-lying $6s$ empty states of the electronegative Bi atom produce empty isolated bands in the gap of the parent materials, effectively lowering the band gap by 1$\sim$2eV in various perovskites. Ferroelectricity (and therefore inversion symmetry breaking) weakens but survives upon doping, which enables the "shift current" mechanism for photocurrent generation, while the decreased band gap helps absorb low energy photons in the visible range. Furthermore, the existence of multiple band gaps allows for solar conversion devices with efficiency beyond the traditional Shockly-Queisser limit, in which successive photon excitations result in carriers with higher energy than a single-step excitation would achieve.

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