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The Optical Band Gap of Perovskite Materials for Solar Cells

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Perovskite thin films $CH_3NH_3PbCl_{3-x}Cl_x$ in this project are deposited by two-step deposition method to study the effect of chloride on the optical band gap. In this experiment, the band gap is insignificantly increased from 1.60 \pm 0.01 eV with no Cl-doping to 1.62 \pm 0.01 eV with 16% Cl-doping because some chloride ions cannot replace the iodide positions in $CH_3NH_3PbI_3$ and form $CH_3NH_3PbCl_3$ instead. Though the crystal structure of $CH_3NH_3PbI_3$ is cubic, with heavily Cl-doping, the crystal structure of $CH_3NH_3PbCl_{3-x}Cl_x$ becomes tetragonal and longer annealing time results in the leaving of Chloride in $CH_3NH_3PbCl_{3-x}Cl_x$. The presence of residual PbI_2 also affects the photon absorption of perovskite.

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