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Effects of copper or germanium additions on the stabilized formation of α-phase formamidinium lead triiodide perovskites

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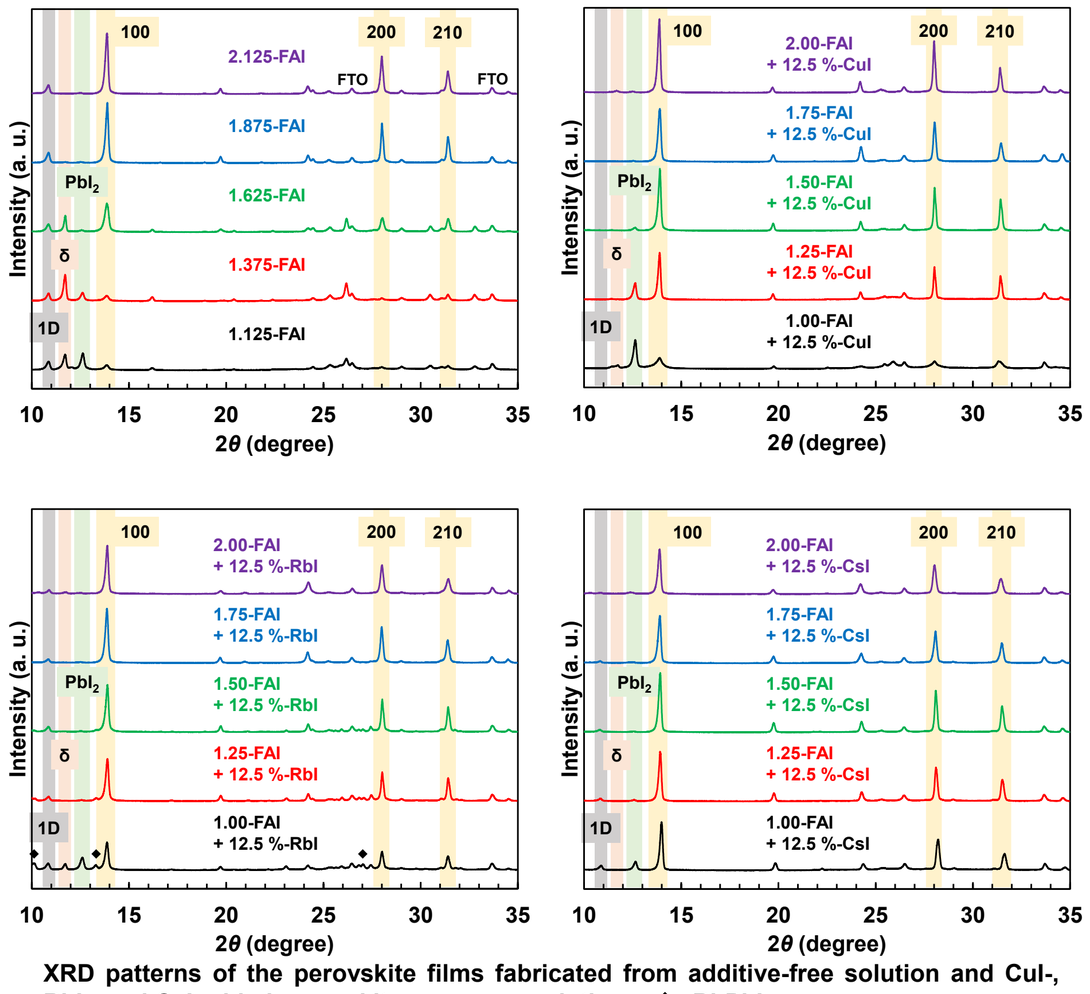
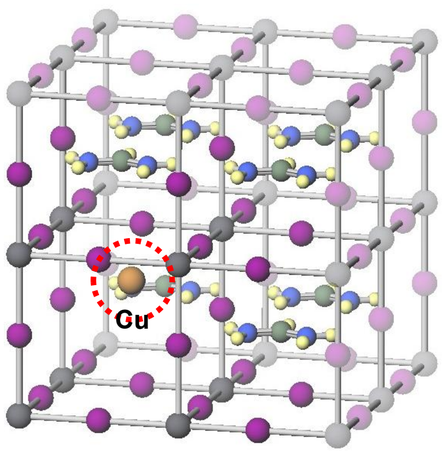
INTRODUCTION & AIM

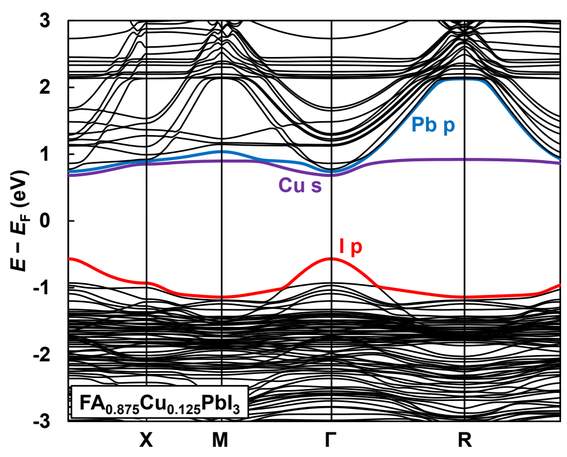
Formamidinium lead triiodide ($FAPbI_3$) is one of the candidate materials for stable perovskite solar cells. There exist optically active cubic α-$FAPbI_3$ phase, optically inactive hexagonal δ-$FAPbI_3$ phase, and one-dimensional phase. Since the δ-phase is thermodynamically stable, the structural phase transition from the α-phase to the δ-phase causes a serious problem on the photovoltaic efficiencies. The aim of this study is to investigate the effects of copper (Cu) or germanium (Ge) additions on the formation of $FAPbI_3$.

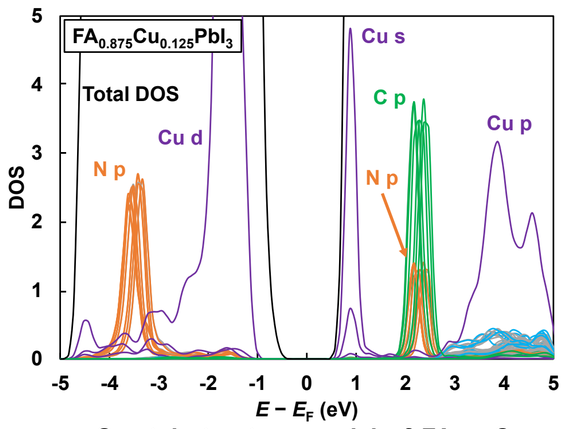
Effects of Cu

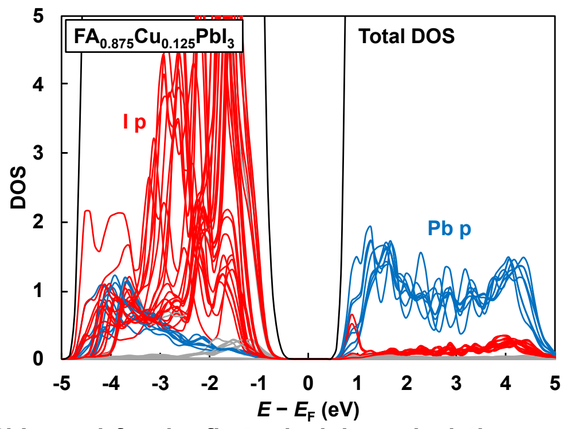


XRD patterns of the perovskite films fabricated from additive-free solution and CuI-, RbI-, and CsI-added perovskite precursor solutions. ◆: $RbPbI_3$.



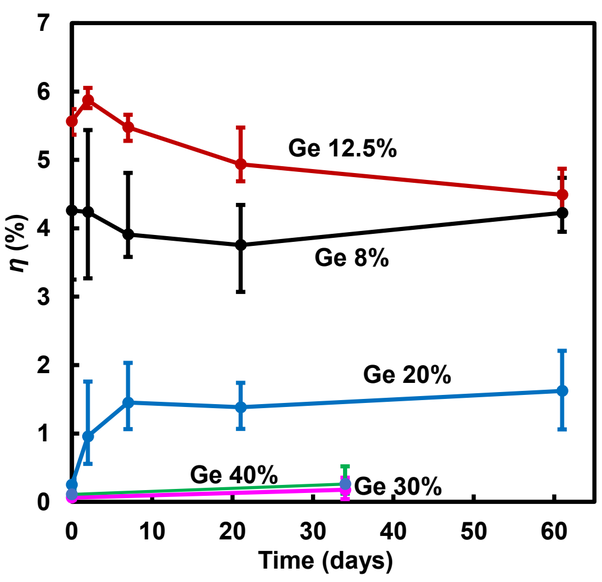


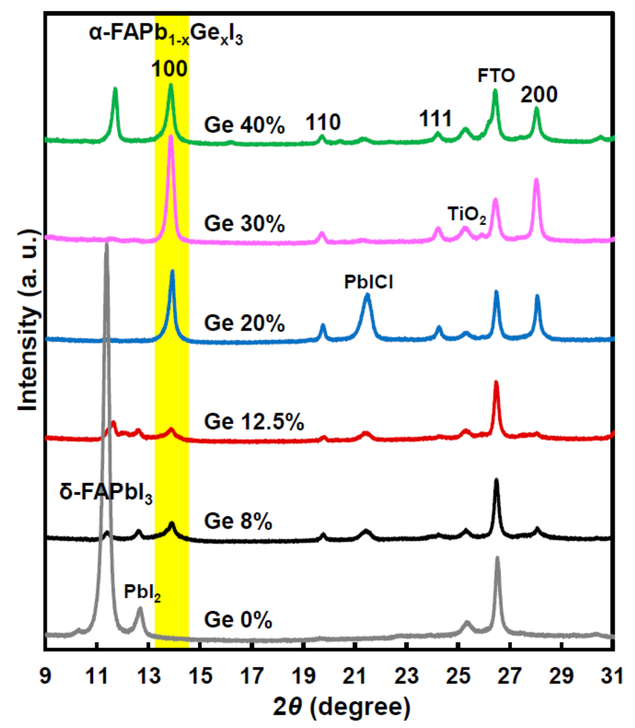




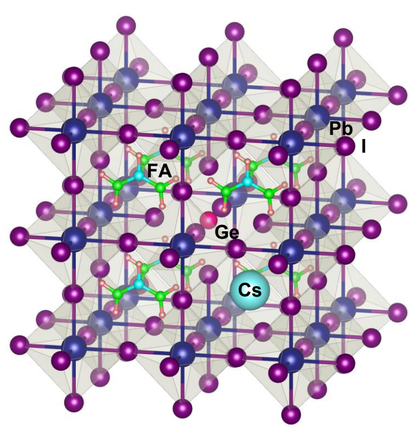
Crystal structure model of $FA_{0.875}Cu_{0.125}PbI_3$ used for the first-principles calculations. Band structure of $FA_{0.875}Cu_{0.125}PbI_3$. pDOS of Cu/N/C and Pb/I.

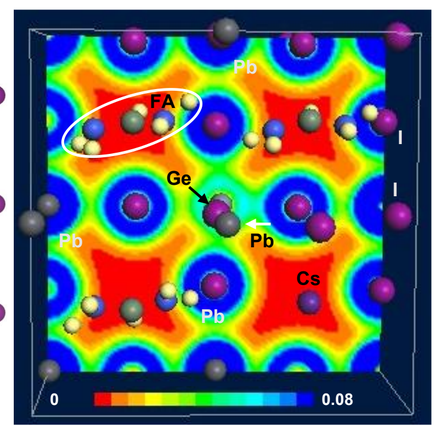
Effects of Ge

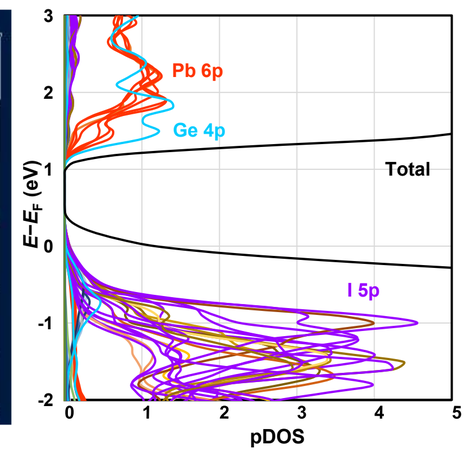




Changes of conversion efficiencies as a function of time. XRD patterns of the present perovskite solar cells.







Structure model, electron density distributions and partial density of states of $FA_{0.875}Cs_{0.125}Pb_{0.875}Ge_{0.125}I_3$.

CONCLUSION

Cu or Ge were added in the present study, as a method for stabilizing the α-phase, to suppresses formation of the δ-phase and one-dimensional phase. When Cu was added at the lead site, diffraction peaks of α-phase increased. Ge addition also increased the diffraction intensity of α-phase and decreased the diffraction intensity of PbI_2. The possibility of stabilization of $FAPbI_3$ by Cu introduction at the FA site was also demonstrated. The first-principles band calculation on the Cu-doped $FAPbI_3$ at the FA site indicated that the total energy value of the crystal decreased. From the calculated partially density of states, the valence band and conduction band are dominated by I-p orbitals and Pb-p orbitals, respectively, and the energy level of the Cu-d orbital is formed at a position slightly lower than the valence band maximum. The effectiveness of Cu introduction in stabilizing the formation of α-$FAPbI_3$ was also demonstrated in the synthesized $FAPbI_3$ crystal.

REFERENCES

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