School of Physical Sciences – Materials for Energy and Electronics (MEE) Group

STABILISATION OF THE PEROVSKITE PHASE OF ALL-INORGANIC MATERIALS FOR PHOTOVOLTAIC APPLICATIONS

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Introduction

Photovoltaic (PV) devices harness solar energy to reduce the dependance on fossil fuels. Current technologies are expensive, and efficiencies have not reached the maximum yet.

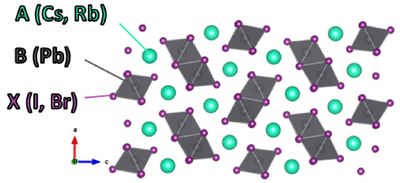
Lead halide perovskites are promising PV materials, with efficiencies > 25%, and competitive with commercial silicon devices. Silicon cells need a high purity and thick films. Perovskites are cheap materials that can be used as thin films and can be obtained via low-cost processes.

All-inorganic lead halide perovskites, $APbX_3$ (A= Cs, Rb; X= I, Br) have good optoelectronic properties and a high thermal stability. Nevertheless, the inorganic A cations are small, and tolerance factors (τ) are low. A low tolerance factor (τ < 0.8) means that, at room temperature, these materials stabilise in a non-perovskite structure, that is also non-photoactive (Table 1).

Table 1: Tolerance factors of the all-inorganic materials

$$\tau = \frac{r\,A\,cation + r\,halide}{\sqrt{2}\,(r\,Pb + r\,halide)}$$

Compound	τ
$CsPbBr_3$	0.862
$CsPbI_3$	0.851
$RbPbBr_3$	0.826
$RbPbI_3$	0.818



Non-perovskite
Non-photoactive
Formed at room temperature

3 approaches to stabilise the perovskite phase:

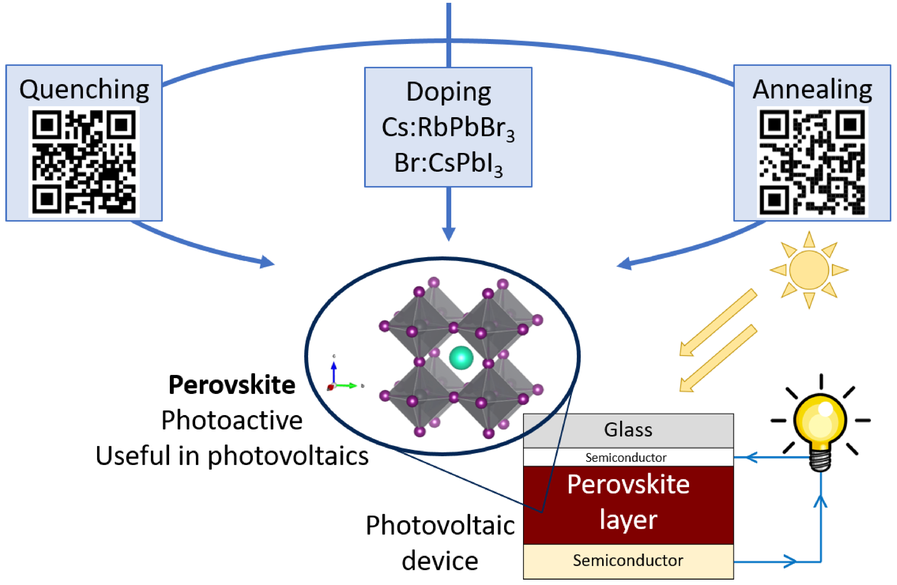


Figure 1: Stabilisation approaches of all-inorganic lead halide perovskites

Method

$CsPbI_3$ and $RbPbBr_3$ were synthesised via self-flux method in the non-perovskite phase. Three approaches were used to stabilise the photoactive perovskite phase at room temperature (RT) (Figure 1):

- **Quenching**: the perovskite phase forms at high temperatures and the rapid cooling down does not allow the structure to go back to non-perovskite.
- **Doping**: increases the tolerance factor and the stability of the perovskite phase at RT. $CsPbI_3$ was doped with Br and $RbPbBr_3$ with Cs.
- **Annealing**: forms the perovskite phase at high temperature and the material stays in that phase when cooling down.

Results

- The perovskite phase of $CsPbI_3$ was stabilised by quenching the non-perovskite sample.
- $RbPbBr_3$ was obtained in the perovskite phase by annealing the non-perovskite sample.
- The doped samples were thermally treated, and the perovskite phase was stabilised for all the intermediate compositions.

All the materials were obtained in the *Pnma* orthorhombic perovskite phase (Figure 2). The three approaches reduced the band gap of the materials, making them suitable for PV applications (Table 2).

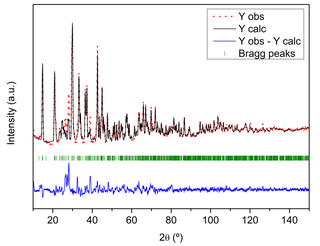


Figure 2: Rietveld refinement of the orthorhombic perovskite phase

Table 2: Lattice parameters and band gaps of the perovskite phase

Compound	a (Å)	b (Å)	c (Å)	Band gap (eV)
$CsPbI_3$	8.8651(4)	12.4817(5)	8.5786(4)	1.73
$RbPbBr_3$	8.3516(8)	11.465(1)	7.8402(6)	2.62

Conclusions

All-inorganic materials were successfully stabilised in the perovskite phase at RT using 3 different approaches. PV perovskite films will reduce the cost of the devices as well as carbon emissions to obtain sustainable, affordable, and clean energy, protecting the future of our planet.

References

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