Erratum: Intrinsic Defect Properties in Halide Double Perovskites for Optoelectronic Applications [Phys. Rev. Applied 10, 041001 (2018)]

Tianshu Li,¹ Xingang Zhao,¹ Dongwen Yang,¹ Mao-Hua Du^{1b},² and Lijun Zhang¹

¹ State Key Laboratory of Superhard Materials, Key Laboratory of Automobile Materials of MOE, and College of Materials Science and Engineering, Jilin University, Changchun 130012, China

² Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

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There is an error in the calculated phase diagram of $\text{Cs}_2\text{AgInCl}_6$ in the paper “Intrinsic Defect Properties in Halide Double Perovskites for Optoelectronic Applications” [Phys. Rev. Applied 10, 041001 (2018)] [1]. The error is caused by the missing of a secondary phase of $\text{Cs}_3\text{In}_2\text{Cl}_9$ (Fig. 2a). The corrected Fig. 2a is shown below.

Corrected FIG. 2(a)

The inclusion of $\text{Cs}_3\text{In}_2\text{Cl}_9$ as a competing phase to $\text{Cs}_2\text{AgInCl}_6$ lowers the maximum In chemical potential ($\Delta\mu_{\text{In}}$) and increases the minimum Ag chemical potential ($\Delta\mu_{\text{Ag}}$) allowed for the growth of $\text{Cs}_2\text{AgInCl}_6$. As a result, the defect formation energies calculated at the In-rich limit [Fig. 3(a)-(b)] and at the Ag-poor limit (Fig. 3(c) and Fig. S1) need to be corrected as shown below.

Corrected FIGs. 3(a-b) and S1.

The correction to the phase diagram leads to an increase of the calculated lowest-attainable Fermi level in Cs₂AgInCl₆, by about 0.1 eV (the crossing point between V_{Cl} and V_{Ag} in Fig. S1), but does not affect the p-type conductivity because the Fermi level is still well below the midgap as shown in Fig. S1. The main conclusions of the paper remain valid.

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- [1] T. Li, X. Zhao, D. Yang, M.-H. Du, and L. Zhang, Intrinsic Defect Properties in Halide Double Perovskites for Optoelectronic Applications, *Phys. Rev. Appl.* **10**, 041001 (2018).