Supporting Information

Highly efficient lead-free (Bi,Ce)-codoped Cs₂Ag_{0.4}Na_{0.6}InCl₆ double perovskites for white LEDs

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Figure S1. Time resolved photoluminescence spectra of $Cs_2Ag_{0.4}Na_{0.6}InCl_6$:X (X = Bi; Bi, Mn; Bi, Ce; Bi, Ni) perovskite phosphors ($\lambda_{ex} = 350$ nm).

| Sample | Designed composition | Measured composition by XPS | Ag/In molar ratio measured by ICP-MS |
|---------------------|--|---|--|
| Bi doped | $Cs_2Ag_{0.4}Na_{0.6}In_{0.99}Cl_6Bi_{0.01}$ | $\begin{array}{c} Cs_{1.92}Ag_{0.22}Na_{0.53}In_{0.99}Cl_{5.68}\\ Bi_{0.016} \end{array}$ | 0.32 |
| (Bi,Mn)- codoped | $Cs_{2}Ag_{0.4}Na_{0.61}In_{0.98}Cl_{6}Bi_{0.01}\\Mn_{0.01}$ | $\begin{array}{l} Cs_{1.79}Ag_{0.21}Na_{0.63}In_{0.98}Cl_{5.62}\\ Bi_{0.015}Mn_{<0.01} \end{array}$ | 0.47 |
| (Bi,Ce)- codoped | $\begin{array}{l} Cs_{2}Ag_{0.4}Na_{0.6}In_{0.98}Cl_{6}Bi_{0.01}\\ Ce_{0.01}\end{array}$ | $\begin{array}{l} Cs_{1.81}Ag_{0.22}Na_{0.71}In_{0.98}Cl_{5.80}\\ Bi_{0.018}Ce_{0.018}\end{array}$ | 0.40 |
| (Bi,Ni)- codoped | $\begin{array}{l} Cs_{2}Ag_{0.4}Na_{0.61}In_{0.98}Cl_{6}Bi_{0.01}\\ Ni_{0.01} \end{array}$ | $\begin{array}{l} Cs_{1.92}Ag_{0.20}Na_{0.65}In_{0.98}Cl_{5.82}\\ Bi_{0.015}Ni_{0.031}\end{array}$ | 0.38 |

Table S1. Comparison of designed composition and measured composition by XPS for each sample.

Table S2. Summary of calculation details for the total formation energies.

| Chemical Formula | Atom Number | Total Energy (E _{total} , eV) | Formation Energy Equations ^{a)} |
|--|---|---|---|
| $Cs_2Ag_{0.4}Na_{0.6}InCl_6$ | $Cs_{40}Ag_8Na_{12}In_{20}Cl_{120}$ | 144897.513 | Referenced energy |
| $Cs_2Ag_{0.4}Na_{0.6}Bi_{0.05}$ | $Cs_{40}Ag_8Na_{12}BiIn_{19}Cl_{120}$ | 145339.653 | E_{total} - E_{ref} - μ_{Bi} + μ_{In} |
| $In_{0.95}Cl_6$ | | | |
| $\begin{array}{l} Cs_2Mn_{0.05}Ag_{0.4}Na_{0.55}\\ Bi_{0.05}In_{0.95}Cl_6 \end{array}$ | $Cs_{40}MnAg_8Na_{11}BiIn_{19}Cl_{120}$ | 146883.112 | $\begin{array}{rrrr} E_{total} & \text{-} & E_{ref} & \text{-} & \mu_{Mn} \\ + \mu_{Na} \text{-} & \mu_{Bi} + \mu_{In} \end{array}$ |
| $\begin{array}{l} Cs_2Ce_{0.05}Ag_{0.4}Na_{0.55}\\ Bi_{0.05}In_{0.95}Cl_6 \end{array}$ | $Cs_{40}CeAg_8Na_{11}BiIn_{19}Cl_{120}$ | 145466.068 | $\begin{array}{rrrr} E_{total} & \text{-} & E_{ref} & \text{-} & \mu_{Ce} \\ _{+}\mu_{Na}\text{-}\mu_{Bi} + \mu_{In} \end{array}$ |
| $\begin{array}{l} Cs_2Ni_{0.05}Ag_{0.4}Na_{0.55}\\ Bi_{0.05}In_{0.95}Cl_6 \end{array}$ | $Cs_{40}NiAg_8Na_{11}BiIn_{19}Cl_{120}$ | 148358.726 | $\begin{array}{rrrr} E_{total} & \text{-} & E_{ref} & \text{-} & \mu_{Ni} \\ + \mu_{Na} \text{-} & \mu_{Bi} + \mu_{In} \end{array}$ |

^{a)} $E_{ref} = -144897.513 \text{ eV}; \ \mu \text{ is chemical potential of an element}, \ \mu_{Bi} = -1865.037 \text{ eV}; \ \mu_{In} = -1423.122 \text{ eV}; \ \mu_{Na} = -1159.212 \text{ eV}; \ \mu_{Ce} = -1283.719 \text{ eV}; \ \mu_{Mn} = -2707.688 \text{ eV}; \ \mu_{Ni} = -4182.087 \text{ eV}.$



Figure S2. Temperature dependency of normalized PL integral intensity (a), emission peak position (b) and FWHM (c) in the temperature range of 85 - 435 K for $Cs_2Ag_{0.4}Na_{0.6}InCl_6$ phosphors doped with 1% Bi; 1% Bi, 1% Mn; 1% Bi, 1% Ce and 1% Bi, 1% Ni.