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Addition/Correction

Correction to "Inorganic Halide Double Perovskites with Optoelectronic Properties Modulated by Sublattice Mixing"

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We recently noticed two errors that have led to an addition and correction to *J. Am. Chem. Soc.* 2020, 142 (11), 5135−5145, DOI: 10.1021/jacs.9b12440. An error in the application of perovskite probabilities, $P(\tau)$, used to select the set of compounds for evaluation artificially excluded 51 compounds from further evaluation. These compounds have now been evaluated in the same manner as the original 311. A second error in data processing led to the exclusion of potential competing phases in the Cs−B−B'−Cl chemical spaces used to compute the stability (ΔH_d) of each compound. The stabilities of affected compounds have been recomputed considering these additional competing phases.

The conclusions published in the original manuscript are unchanged, and the addition of 51 compounds to the data set further emphasizes the potential for new materials discovery in this chemical space with the number of materials predicted to be nontoxic and (meta)stable and have desirable band gaps for optoelectronic applications increasing from 47 in the originally published version to 55 with the Addition and Correction. Revised versions of Figure 2, Table S1, an interactive version of Figure 2 (in the SI), and a downloadable version of Table S1 (in the SI) are provided here. These figures and tables contain the calculated stabilities and band gaps of all 362 compounds.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/jacs.0c08740.

Revised version of Table S1: list of all $Cs_2BB'Cl_6$ compounds screened in this study sorted by their B and B' cations (PDF)

Interactive version of Figure 2 (ZIP)

Downloadable version of Table S1 (TXT)

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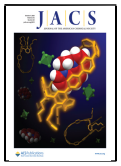

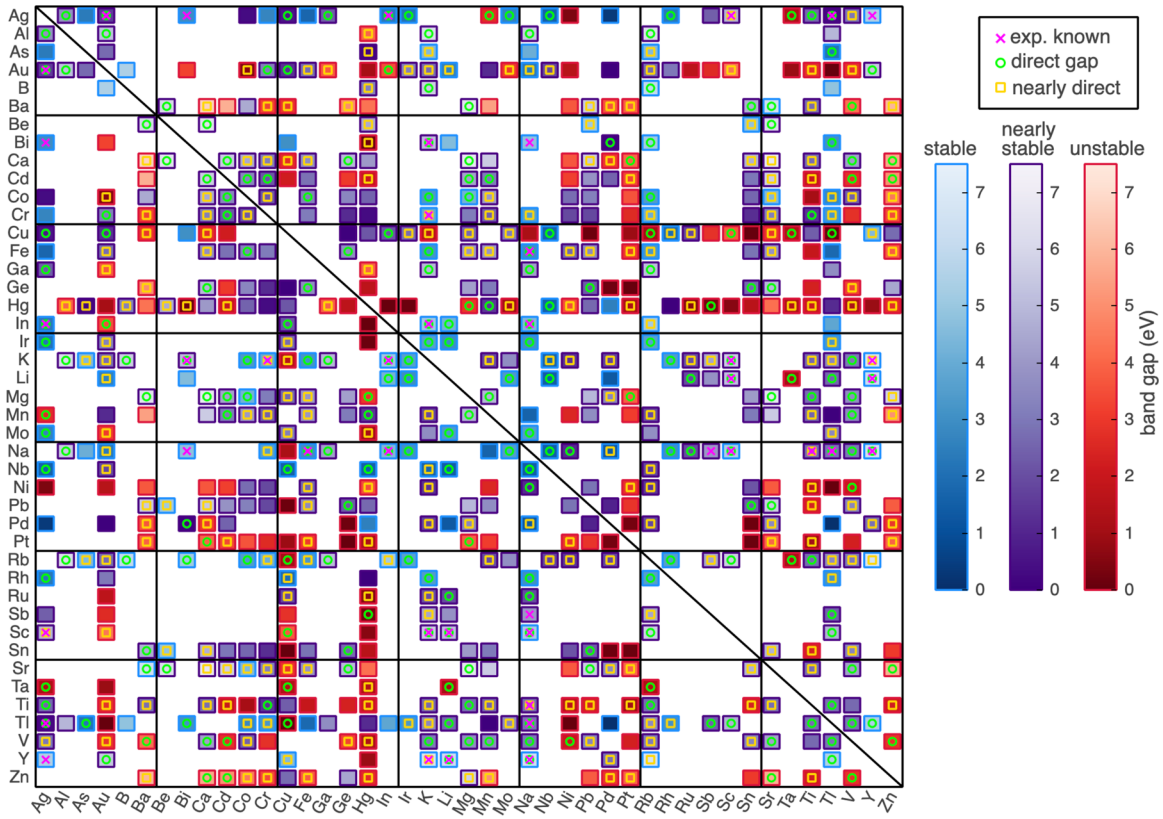

Figure 2. Map of $Cs_2BB'Cl_6$ properties. B and B' are defined along each axis (note that B and B' are treated equivalently in this work; therefore, the data are mirrored across the diagonal line). Stable compounds ($\Delta H_d \leq 0$ eV/atom) are shown in blue, nearly stable compounds ($0 \leq \Delta H_d < 0.05$ eV/atom) are shown in purple, and unstable compounds are shown in red ($\Delta H_d > 0.05$ eV/atom), where ΔH_d is calculated with SCAN. The color intensity of each compound corresponds to the band gap calculated using single-point HSE06 at the SCAN-optimized geometry (spHSE06@SCAN). Compounds that have direct band gaps are indicated with an open green circle. Compounds that have indirect gaps that are within 100 meV of the direct gap are indicated with an open gold square. Compounds that have been reported experimentally are indicated with a pink ×. An interactive version of this plot that assists with navigation and displays additional properties is available in the Supporting Information.

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