(U)Mapping the chemical landscape of Halide Double Perovskites

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Halide Double Perovskites (HDPs) are quarternary materials with chemical formula A2BB'X6, which have recently been regaining scientific attention because they show beneficial properties for photovoltaic, X-ray detection, sensing, photocatalysis, and spintronic applications. However, with over 40.000 potential HDP compositions, much of the available landscape remains underexplored. For this, we have generated a database of spin-polarized, hybrid functional (HSE06) DFT electronic structure data, combined with an in-depth chemical bonding analysis using LOBSTER [1]. This was done for all HDPs with Cesium on the A-site and that are predicted to be stable by Bartel's tolerance factor [2], resulting in a database of quantum-chemical data on ~2600 HDP compositions. The database features some interesting findings, e.g., 134 predicted half-metals. We also used dimensionality reduction (UMAP) to visualize the data and highlight underlying trends, which can be explored in an interactive platform. Furthermore, the database of high-quality quantum-chemical data covering the entire chemical landscape serves as a valuable resource for discovering new halide perovskites using data-driven and machine learning techniques.

References

[1] www.cohp.de
[2] C.J. Bartel, C. Sutton, B.R. Goldsmith, R. Ouyang, C.B. Musgrave, L.M. Ghiringhelli, M. Schefler, Sci. Adv. 5, 2, (2019) eaav0693 DOI: 10.1126/sciadv.aav0693

Figures

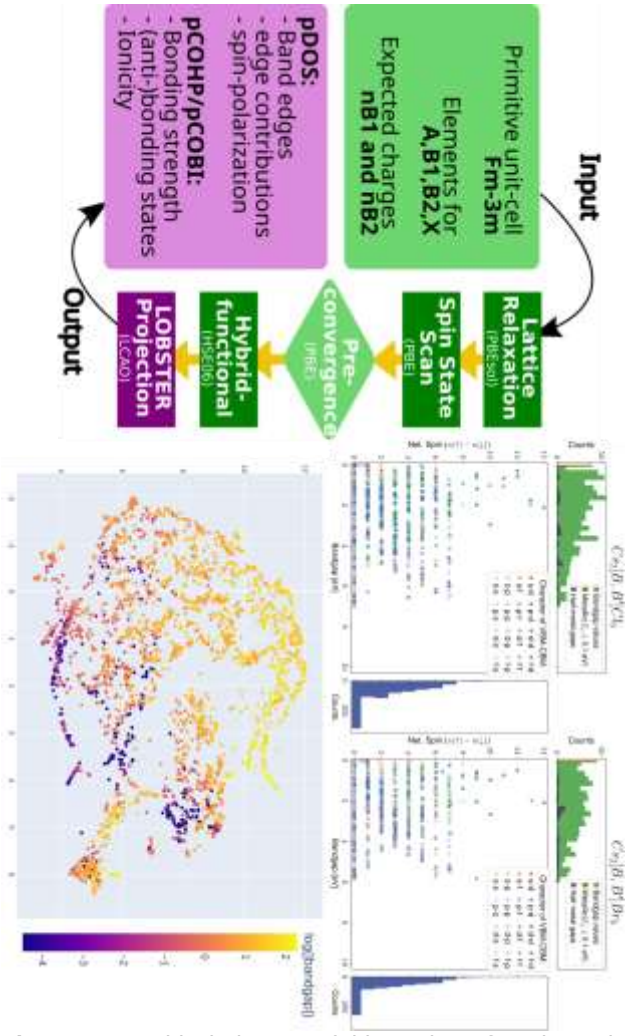

Figure 1. Graphical abstract of this work. **Left:** schematic of the workflow. **Top right:** Scatter plots of net spin vs. bandgap values found for the chloride HDPs (on the left) and bromide HDPs (on the right). **Bottom right:** UMAP projection based on the B-site pDOS's (metric: Bray-Curtis, n_neighbours=5, min_dist=0.1), the coloring is based on the logarithm of the bandgap values.