

Supporting Information

Harness Engineered LLM Agents for Material Science: A Case Study on Perovskite Materials with Machine Learning and Materials Project

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KEYWORDS Harness Engineering; agent; large language model; LLM; perovskite materials

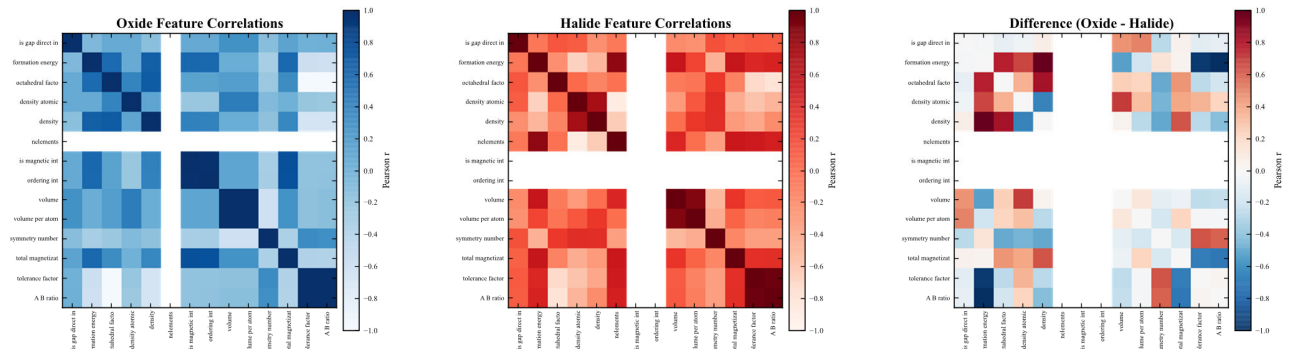


Figure S1. Feature correlation comparison map between Oxide and Halide subclasses. (a) Oxide correlation matrix. (b) Halide correlation matrix. (c) Difference matrix (Oxide minus Halide). Constant features with zero variance within a subclass are displayed in the matrices for completeness. These features contain no within-subclass variation and therefore cannot contribute to within-subclass regression.

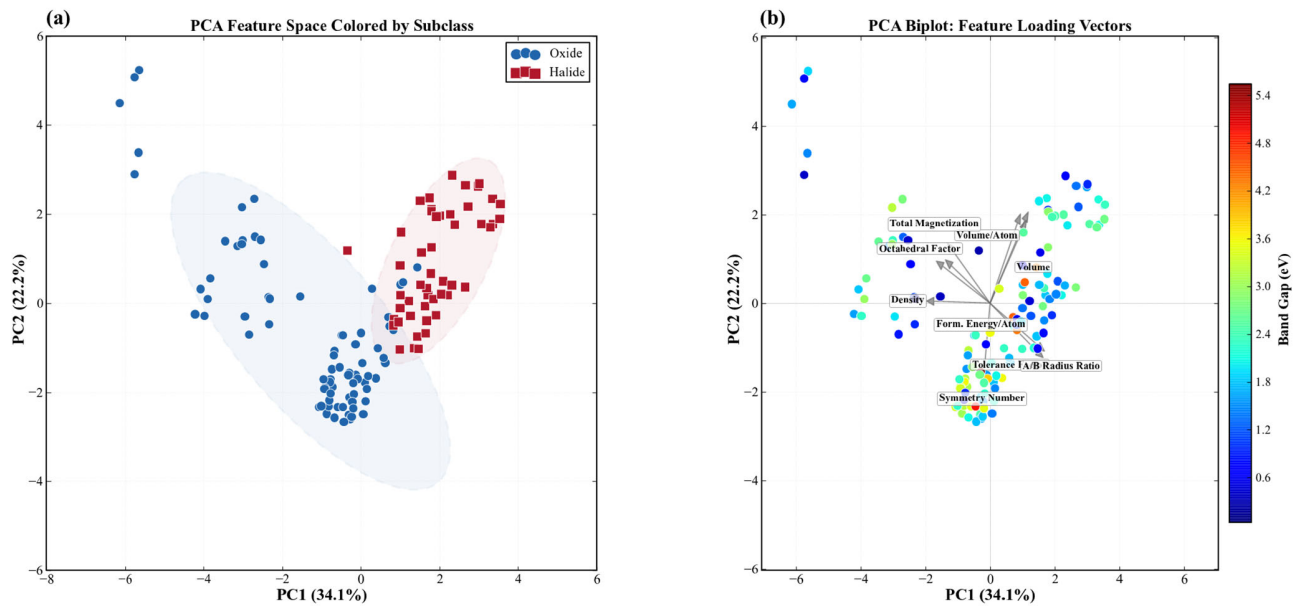


Figure S2: PCA projection of the 14-dimensional perovskite descriptor space. (a) Samples colored by subclass: oxide (blue circles) and halide (red squares) perovskites occupy largely non-overlapping regions in the PC1–PC2 plane. The separable distributions support the expert-

defined oxide/halide partition as an initial modeling hypothesis, but they do not show that this partition is optimal or that it was discovered automatically. In a future adaptive Harness workflow, the same descriptor-space evidence could be combined with matched prediction feedback to compare expert rules, clustering solutions, learned representations, and hierarchical taxonomies. (b) The same projection colored by band gap (eV), overlaid with feature loading vectors (gray arrows). Arrow direction and length indicate the contribution of each descriptor to PC1 and PC2.

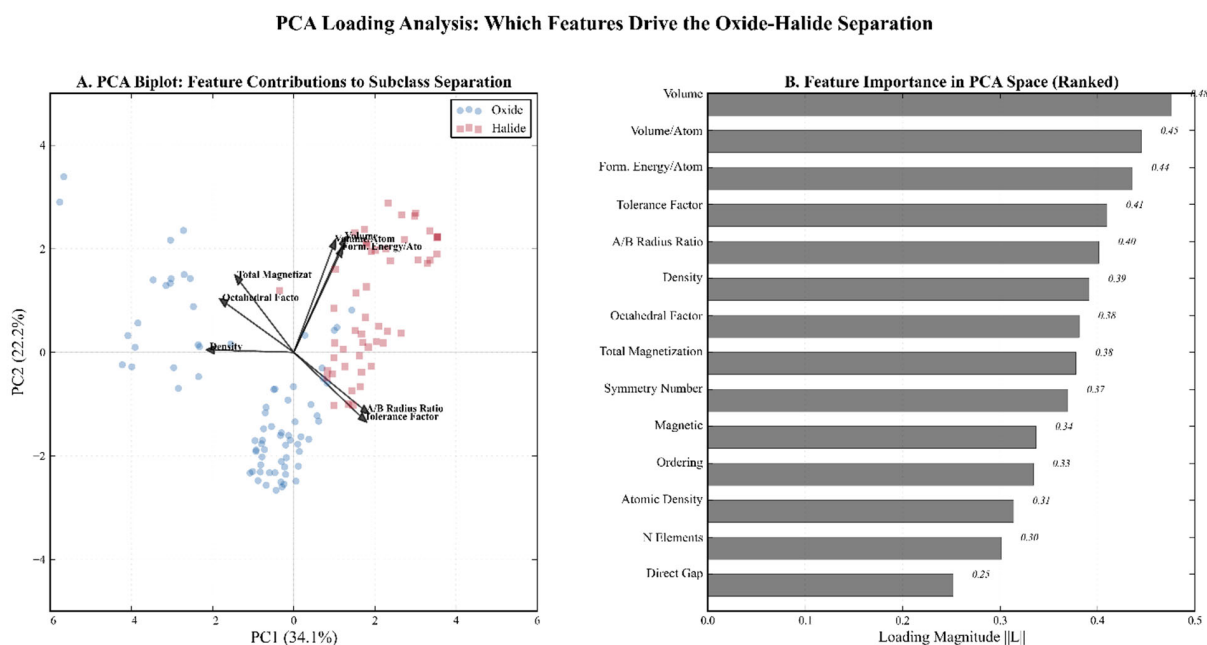


Figure S3: PCA loading analysis for the 14-dimensional perovskite descriptor space (gradient boosting). (a) Biplot showing the PCA projection with subclass differentiation (blue circles: oxide; red squares: halide) overlaid with the top eight feature loading vectors (black arrows). Arrow direction and length indicate the contribution of each descriptor to PC1 and PC2. (b) Ranked feature importance in PCA space for the descriptors.