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Accelerated Materials Discovery with Machine-Learning and DFT

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Lead-free double perovskites with the composition A2BB'X6 have emerged as a promising new class of materials for photovoltaic applications as alternative to the lead- containing halide perovskites. They are stable for a wide range of chemical compositions on the different sublattices, which allows tuning of desired properties. However, efficient exploration of this enormous chemical space requires innovative machine-learning and high-throughput methods. In a first example we considered only two elements in different ratios on both sublattices B and B'. By using a Minimum Redundancy Maximum Relevance (MRMR) feature selection algorithm and Gaussian Process Regression (GPR) we show that important photophysical parameters such as recombination rates and Stokes shifts can be predicted from a large data set of ground state properties, which was generated by high-throughput DFT calculations [1]. Next, we allowed many different elements on all sublattices to create so-called high entropy compositions with increased thermodynamic stability due to the gain of configurational entropy. A Sobol sequence is used to generate a minimal set of representative combinations capable of describing the broader compositional space. By combination with a Trust Region Bayesian Optimization (TuRBO), subsequent iterations are efficiently guided, reducing the computational load from thousands of calculations to mere hundreds. This streamlined approach allows us to identify compositions for well-behaved semiconductors with optimized band gap and effective electron and hole masses, providing a powerful pathway for accelerating the discovery of high-performance, lead-free double perovskites.

[1] M.S. Günthert, L. Lüer, O. Stroyuk, O. Raievska, C. Kupfer, A. Osvet, B. Meyer, C.J. Brabec, Digital Discovery 5 (2026) 1215–1227.