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Machine learning bandgaps of double perovskites[1] GHANSHYAM PILANIA, Los Alamos Natl Lab, ARUN MANNODI-KANAKKITHODI, University of Connecticut, BLAS UBERUAGA, Los Alamos Natl Lab, RAMPI RAMPRASAD, University of Connecticut, JAMES GUBERNATIS, TURAB LOOKMAN, Los Alamos Natl Lab — The ability to make rapid and accurate predictions of bandgaps for double perovskites is of much practical interest for a range of applications. While quantum mechanical computations for high-fidelity bandgaps are enormously computation-time intensive and thus impractical in high throughput studies, informatics-based statistical learning approaches can be a promising alternative. Here we demonstrate a systematic feature-engineering approach and a robust learning framework for efficient and accurate predictions of electronic bandgaps for double perovskites. After evaluating a set of nearly 1.2 million features, we identify several elemental features of the constituent atomic species as the most crucial and relevant predictors. The developed models are validated and tested using the best practices of data science (on a dataset of more than 1300 double perovskite bandgaps) and further analyzed to rationalize their prediction performance.

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