# ML prediction of photoluminescence from high-throughput density functional theory ground state properties on the example of $Cs_2Ag_xNa_{1-x}Bi_yIn_{1-y}Cl_6$

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Lead-free halide double perovskites (LFHDP) have been an emerging material class for various applications in the field of optoelectronics over the last couple of years due to their environmental friendliness and exceptional stability.[1-2] The material class can be enlarged even further by substituting the $Pb^{2+}$ ion not only with one $M^{1+}$ and one $M^{3+}$ ion but with two of each.[3-4] This adaption increases the number of possible materials immensely and gives rise to the demand for a different approach in material investigation: high-throughput (HTP) screening. HTP screening aims to analyze a vast material range in a reasonable time by applying automation techniques and the restriction to swift measurement methods. Overcoming this issue can be done by applying not only HTP experimental methods but also HTP computational methods. Density functional theory (DFT) is able to examine a perfectly controlled range of material compositions for complementary features. The combination of these strategies is a promising approach towards a HTP screening in novel materials discovery and is shown to be applicable on the example of $Cs_2Ag_xNa_{(1-x)}Bi_yIn_{(1-y)}Cl_6$. DFT has access to features like e. g. the lattice parameter, elastic properties and electronic properties whereas experimental methods investigate e. g. optical and vibrational material properties. Using the variety of ion combinations in this LFHDP structure with interchangeable ion ratios opens up a whole new field of materials which can be evaluated by the methods developed on the example of $Cs_2Ag_xNa_{(1-x)}Bi_yIn_{(1-y)}Cl_6$ and therefor to build up a database. Using machine learning algorithms on this database can lead to a deeper understanding of the coupling between the ion exchange and macroscopic material properties. This has be done by a minimum redundancy maximum relevance algorithm embedded in a Gaussian Process Regression to predict the photoluminescence characteristics of $Cs_2Ag_xNa_{(1-x)}Bi_yIn_{(1-y)}Cl_6$.[5]

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