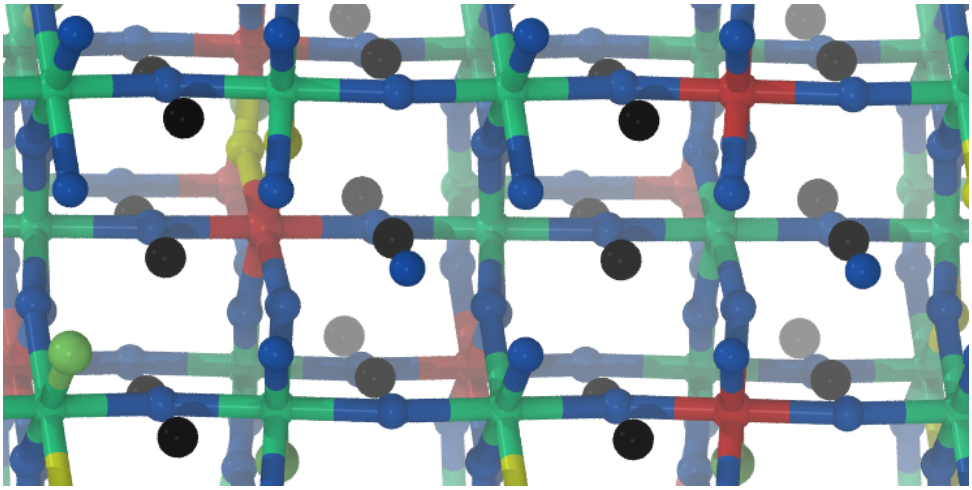
# MASTER THESIS PROJECT

## Towards more efficient solar cells: modelling of band gaps of mixed halide perovskites

By 2050, a quarter of global power generation is hoped to come from solar devices (either solar-to-electricity or solar-to-fuel conversion). Solar cells based on metal halide perovskites show very promising photovoltaic properties with power conversion efficiencies improving rapidly over the last few years and now exceeding 25%. The general chemical formula for halide perovskites is $ABX_3$, where the A-site is occupied by a monovalent cation (organic or inorganic), the B-site by a metal element, and the X-site by a halogen. One of strategies to make halide perovskites more stable and efficient is A, B, or X-site mixing.



Band gap of a semiconductor is one of the main indicators of how well it can absorb light. It has been shown that the band gaps of halide perovskites can be efficiently tuned by mixing their composition. The aim of this project is to **study the band gaps of the mixed compounds**. Within the project, models of mixed halide perovskites will be first generated, using **cluster expansion methods based on machine learning**. Subsequently, electronic properties of the models will be studied using **advanced electronic-structure techniques**.

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