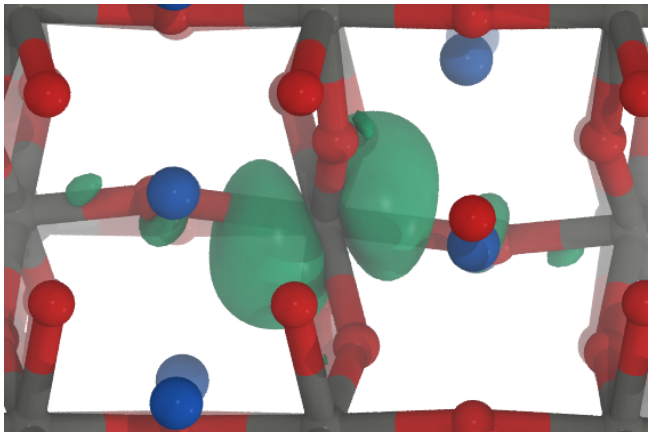
MASTER THESIS PROJECT

Ab initio modelling of small polarons in 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 the strategies to make halide perovskites more stable and efficient is A, B, or X-site mixing.



Due to their complex structure, mixed halide perovskites are much less studied than their simpler (unmixed) counterparts. The aim of this project is to **study the properties of excess charges in the mixed compounds**, in particular charge localization and polaron formation. Within the project, models of mixed halide perovskites will be first generated, using **cluster expansion methods based on machine learning**. Subsequently, excess charges will be introduced to selected models and studied using **advanced electronic-structure techniques**.

If you are interested in the project, please contact Asst. Prof. Julia Wiktor (julia.wiktor@chalmers.se) or Prof. Paul Erhart (erhart@chalmers.se) in the Condensed Matter and Materials Theory division at the Department of Physics.