DFT has proved to be a powerful tool to investigate, otherwise inaccessible, properties of materials. In our past work we considered different properties of methylammonium lead iodide including band structures, vibrational properties, and phase diagram[1,2].

The most recent research in the field aim to reduce or substitute the presence of lead. One viable way to do so it the design of double perovskites. Such structure have general structure ABB'X3, where B and B' are two different metals, as for instance K and Bi.

In collaboration with the experimentalist we employ DFT to predict and design the synthesis of new materials. We primary investigate the behaviour of completely inorganic perovskites as CsAgBiCl3 and CsAgBiBr3. We explored their vibrational space, and predict the existence of different phases using the quasi-harmonic approximation. The same methodology has been extended to the equivalent hybrid perovskites CH3NH3KBiCl3 where our results have been compared with experimental measurements.

Computational methods also allow to design new materials with the perovskites motif before their synthesis, in order to optimise and optimise the synthesis. In our case we consider the bifluoride family with general composition RZnF2H (where R is an organic cation). We considered different compositions in order to investigate which cations could be more stable in such a crystal.