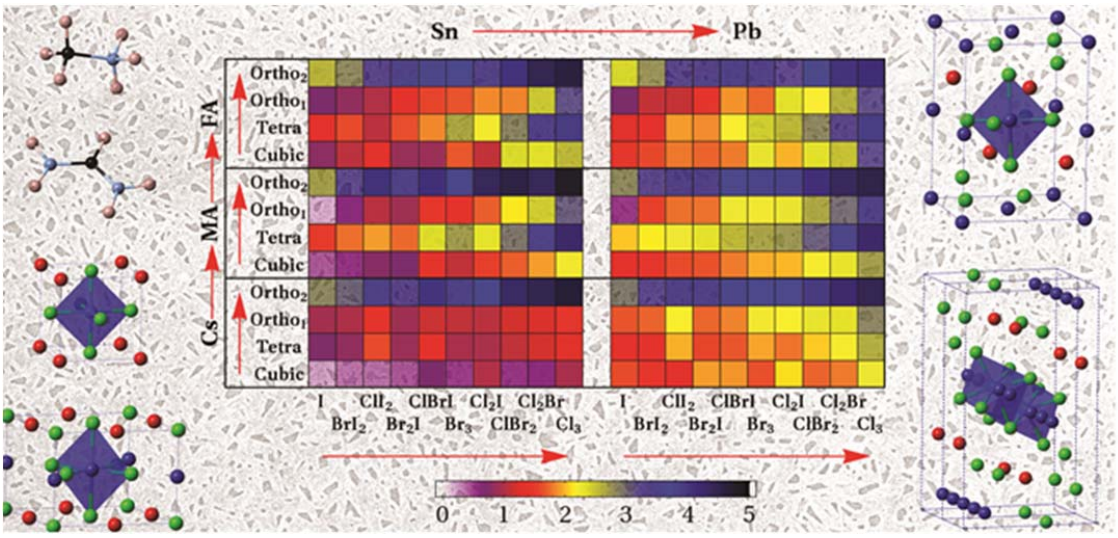
Computational screening of materials for Emergent Solar Cells technologies

Challenge: The advancement of low cost photovoltaics (PV) is a key step towards clean future energy technologies. There are three main families of PV technologies, namely, silicon-based (1st PV generation), thin-film-based (2nd PV generation), and the 3rd PV generation, which includes all the new emergent technologies as organic polymers, dye-sensitized and organic perovskite PV. Today, the silicon-based PV market is completely dominated by China and the thin-film-based is based upon toxic and/or rare elements. 3rd PV generation appears as a promising alternative for European manufactures. However the efficiency of 3rd generation PVs needs to be improved before the can compete in equal ground with the 1st and 2nd PV generations.

Idea: To improve the efficiency of solar cells based on these 3rd PV generation technologies further it is natural to resort to computational methods that allow for fast exploration of the vast space of material composition and structures. Thanks to the enormous growth in computer power, high-throughput computational screening is rapidly becoming an essential tool for accelerated materials discovery and has recently been applied within a wide range of areas.

Your task: You will carry out a computational screening of organic perovskites of materials for 3rd PV generation technologies.



Screening of bandgaps of organic perovskites in different phases.

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