Data Driven Design of Perovskites

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Goal: finding the optimal formula for the hybrid organic inorganic perovskites (HOIPs) for solar cell energy conversion by using statistical models to analyze scattered data in published articles.

Introduction: In recent years, there has seen a rapid emergence of new class of solar cell based on HOIPs, which is a shown . Incorporating perovskites into semiconductor devices such as solar cells has shown good performance. Although the first efficient solid-state perovskite cells were reported in 2012, a very fast progress was made during five years with power conversion efficiencies (PCE) reaching a confirmed 20%. [1]

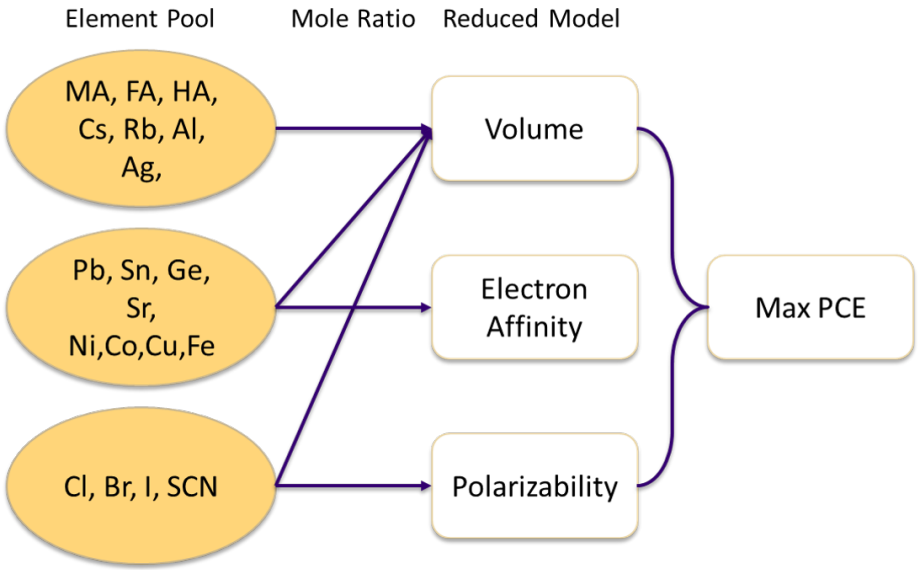

Fig 2. Overview of the layout of the data input for the workflow

Methodology: Because an universal data base of perovskites does not exist yet, we searched through papers from 2015 to 2017. The data from these papers are described in Fig 2. The limited amount of data that we could obtain and the surface curvature complexity still provided a best fitting quality of 0.58.

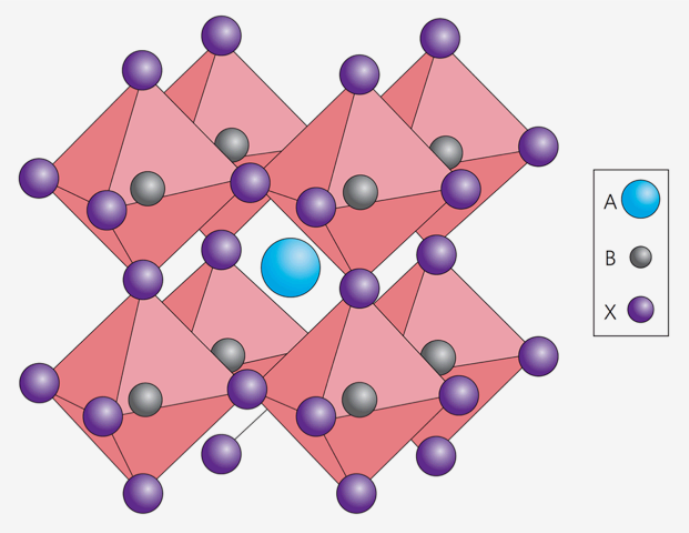

Fig. 1 The schematic structure of a ABX_3 HOIP. Typical HOIP have cations as A sites, Pb^{2+} as the B site element and halogens as X sites.