Using datamining to understand defect mitigation in lead halide perovksites

Alexandre Py[1], Pallavi Singh[2], David Cahen[2], Philip Schulz[1] and Jean-François Guillemoles[1]

[1] CNRS, Ecole Polytechnique, Institut Photovoltaïque d'Ile-de-France UMR 9006, 30 RD 128, 91120 PALAISEAU, France

[2] Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot 76100, Israel

Recent studies demonstrated that halide perovskites (HaPs), display a high degree of structural disorder [1] combined with optoelectronic properties usually associated with crystalline semiconductors such as long carriers lifetime [2]. Does this class of materials (dynamically disordered) tend to minimize structural defects and how do these defects affect the optoelectronic properties of the materials? In this study, we are looking for answers to this challenging question by using data mining approaches to investigate the physical properties of lead HaPs compared to other semiconductors. The aim is twofold:

- Try and identify physical properties (such as thermal conductivity for instance) that distinguish HaPs from other semiconductors;
- Identify materials that display physical properties close to those of HaPs.

We probed a range of physical properties and managed to identify four properties for which halide perovskites distinguish themselves from other semiconductors: linear thermal expansion coefficient, thermal conductivity, isothermal bulk modulus and microhardness. We demonstrate that lead HaPs are soft materials, with very low thermal conductivity compared to other semiconductors. Our conjecture comprises that materials exist in these specific regions of the corresponding Ashby diagrams associated with lead HaPs, which display similar responses for other physical properties, less accessible with datamining (self-healing, sharp absorption coefficients, …). Based on this hypothesis, we define acceptable ranges for each property to scan the database and literature sources for potential candidate materials. We thus put forward a selection of semiconductor compounds to be further explored experimentally to prove (or disprove) our hypothesis.

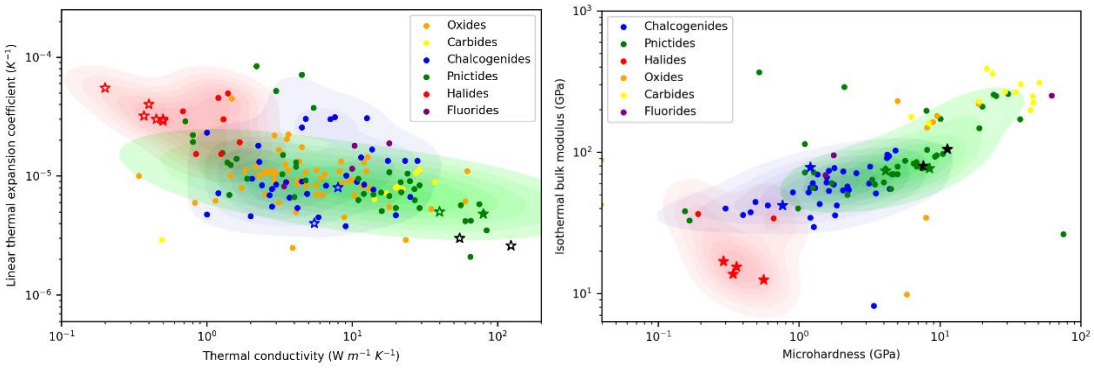

Figure 1: Linear thermal expansion coefficient vs thermal conductivity (resp isothermal bulk modulus vs microhardness) for semiconductors, dots are data taken from the MPDS database. The stars represent compounds of reference (for halides in red, lead HaPs such as $MAPbI_3$, $CsPbI_3$, $MAPbBr_3$, …) with each color attributed to a specific anion group. Si and Ge are labeled in black as they are unary compounds and thus do not fall in our classification with respect to anions. These data come from a literature search when data were not available from the MPDS database (especially true for semi-organic lead HaPs, absent from the database).

[1] Y. Guo, O. Yaffe, T.D. Hull, J.S. Owen, D.R. Reichman, and L.E. Brus, ArXiv (2018).

[2] D.A. Egger, A. Bera, D. Cahen, G. Hodes, T. Kirchartz, L. Kronik, R. Lovrincic, A.M. Rappe, D.R. Reichman, and O. Yaffe, Adv. Mater. **30**, 1800691 (2018).