**Supplementary Information**

**Mechanical Properties of APbX3 (A=Cs or CH3NH3; X=I or Br) Perovskite Single Crystals**

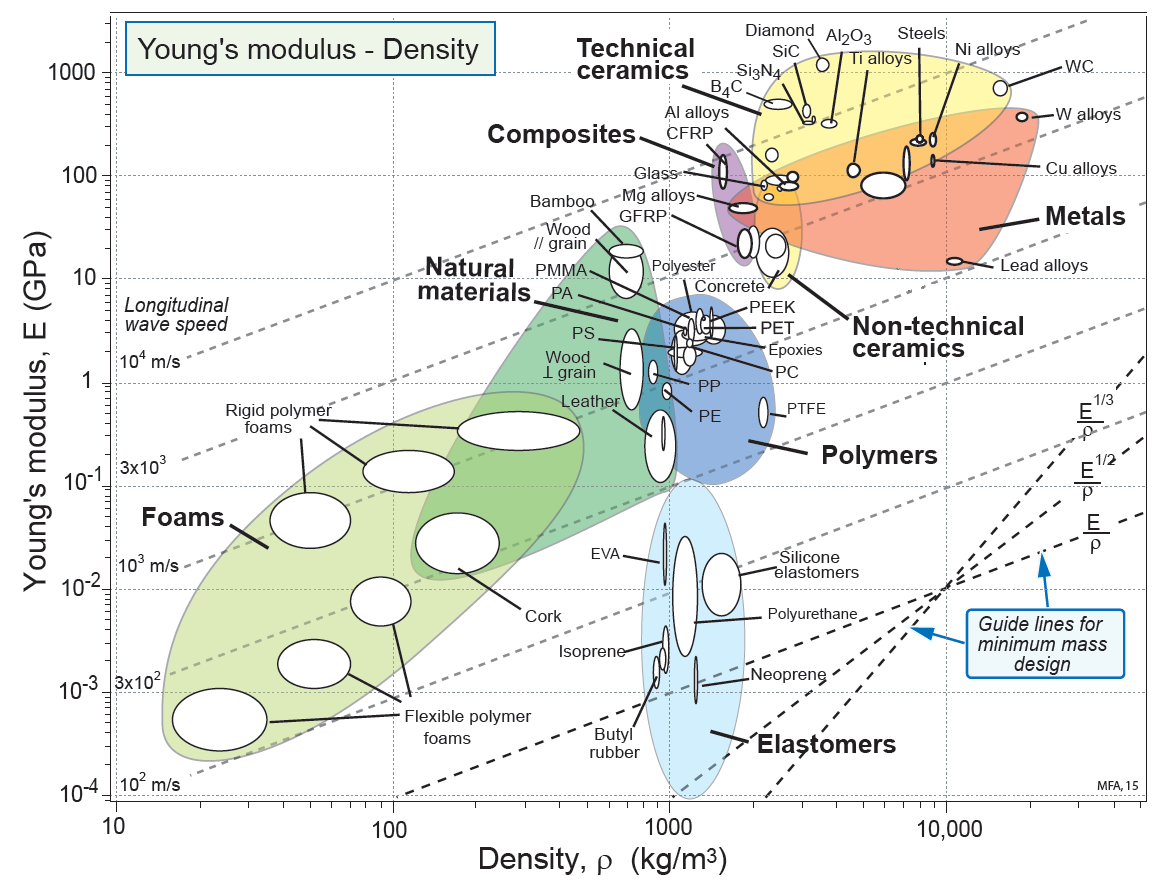
Yevgeny Rakita,Sidney R. Cohen\* †, Nir Klein Kedem, Gary Hodes, David Cahen\*

Materials and Interfaces Department and †Surface Science Laboratory (Chemical Research Support),

Weizmann Institute of Science, Rehovot. 76100, Israel

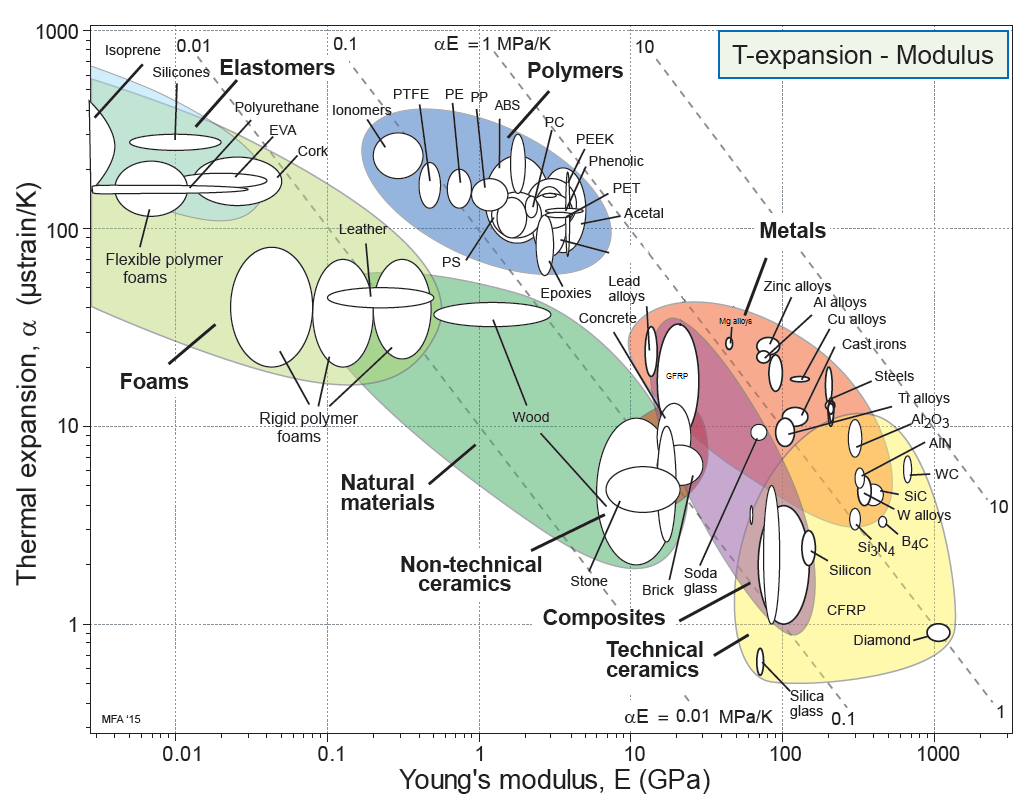
*\* corresponding authors:* [*sidney.cohen@weizmann.ac.il*](mailto:sidney.cohen@weizmann.ac.il) *;* [*david.cahen@weizmann.ac.il*](mailto:david.cahen@weizmann.ac.il)

**Figure S1**: Characteristic Load vs. Displacement curves of APbX3 crystals. The number in the round parenthesis indicates the crystallographic plane facing the indenter.

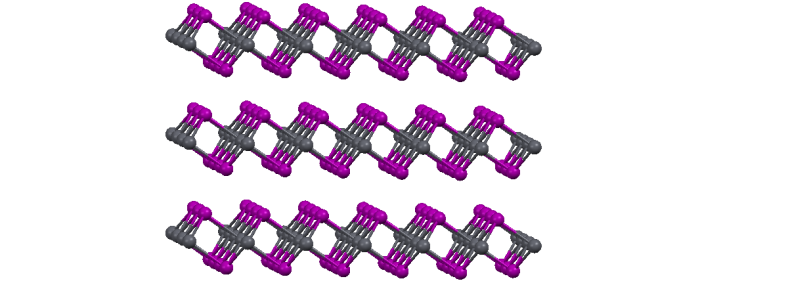


**Lead alloys**

**Figure S2**: Ashby 2D map: density vs. Young’s modulus. Experimentally derived values (from this work or other cited works – see Table 1) are added in the area, designated “ABX3” to which the arrow points: **Red** - CH3NH3PbBr; **Black** - CH3NH3PbI3; **Yellow** - CH3NH3SnI3; **Orange** - CsPbBr3; **Green** - CsPbI3; **Magenta** – PbI2 ; **Blue** – PbBr2. Reprinted with permission from Ashby, M. F. *Materials Selection in Mechanical Design, Fourth Edition*. (Elsevier/ Butterworth-Heinemann, Amsterdam, 2011).



**Figure S3**: Ashby 2D map: linear thermal expansion coefficient vs. Young’s modulus. Experimentally derived values (from this work or other cited works – see Table 1) are added in the area, designated “ABX3” to which the arrow points: **Red** - CH3NH3PbBr; **Black** - CH3NH3PbI3; **Orange** - CsPbBr3; **Magenta** – PbI2; **Blue** – PbBr2. Reprinted with permission from Ashby, M. F. *Materials Selection in Mechanical Design, Fourth Edition*. (Elsevier/ Butterworth-Heinemann, Amsterdam, 2011).



Weak I-I VdW

**strong I-Pb  
(mostly) ionic bond**

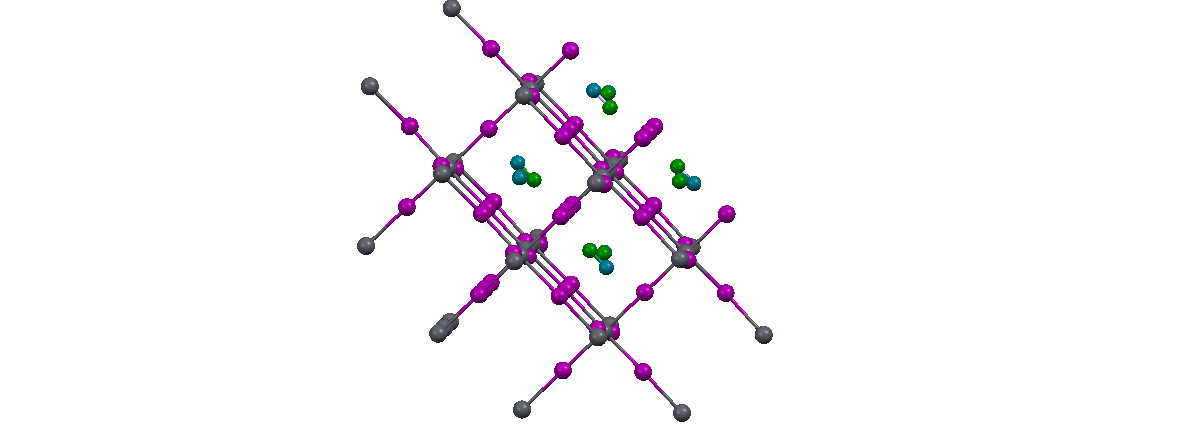
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**c axis**

**c(0001) plane**

**PbI2**

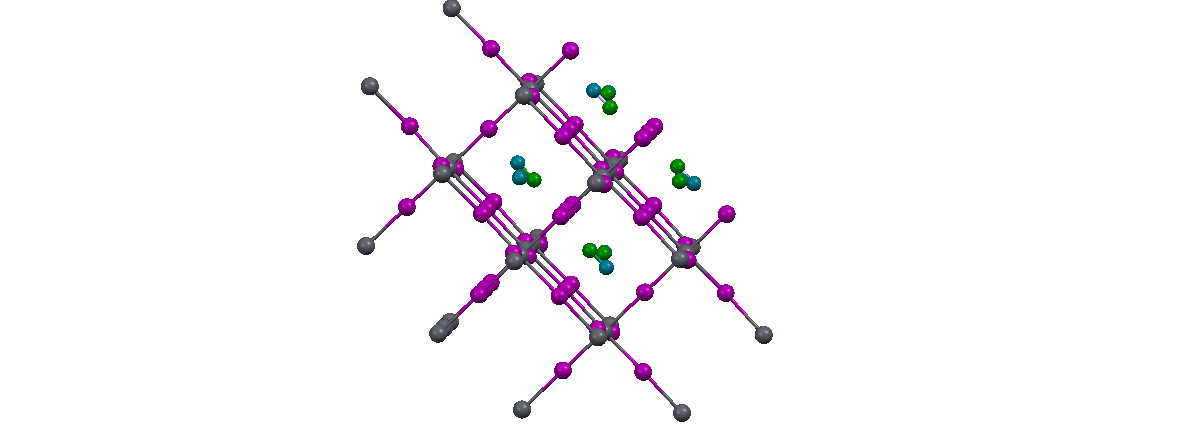
**CH3NH3PbI3**



**c**

**a**

**b**



**c**

**a**

**I**

**Pb**

**C**

**b**

**N**

**Figure S4**: Ball-and-stick crystal structure representation of (top) PbI2 and (bottom) CH3NH3PbI3, illustrating the close relation between the Pb-I in the c(0001) plane and in CH3NH3PbI3.

**Table S1**: Values for Figure 3.

|  |  |  |
| --- | --- | --- |
|  | B-X bond distance (@ RT) [Å] | K [GPa] |
| CH3NH3PbI3 | 3.16 | 12.2 |
|  |  |  |
| CH3NH3PbBr3 | 2.97 | 15.6 |
|  |  |  |
| CH3NH3PbCl3  CH3NH3SnI3 | 2.86  3.13 | 16.5 \*  12.6 |
|  |  |  |
| CsPbI3 | 3.23 | 19.8 |
|  |  |  |
| CsPbBr3 | 2.96 | 15.5 |
|  |  |  |
| MgSiO3 | 1.64 | 264 |
|  |  |  |
| SrTiO3 | 1.95 | 183 |
|  |  |  |
| GdMnO3 | 2.03 | 190 |
|  |  |  |
|  |  |  |
|  |  |  |
| PbBr2 | 3.14 | 23.5 |
|  |  |  |
| c-plane PbI2 | 3.23 | 16.7 |

\* the bulk modulus of CH3NH3PbCl3 was estimated using the measured Young’s modulus of the (100) plane from Ref. 19 (see below), 19.8 GPa, and assuming a Poisson ratio of 0.3.

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*Ref.19: Sun, S., Fang, Y., Kieslich, G., White, T. J. & Cheetham, A. K. Mechanical properties of organic–inorganic halide perovskites, CH3NH3PbX3 (X = I, Br and Cl), by nanoindentation. J. Mater. Chem. A,* *.* ***6,*** *2622–2628 (2015). doi:10.1039/C5TA03331D*