

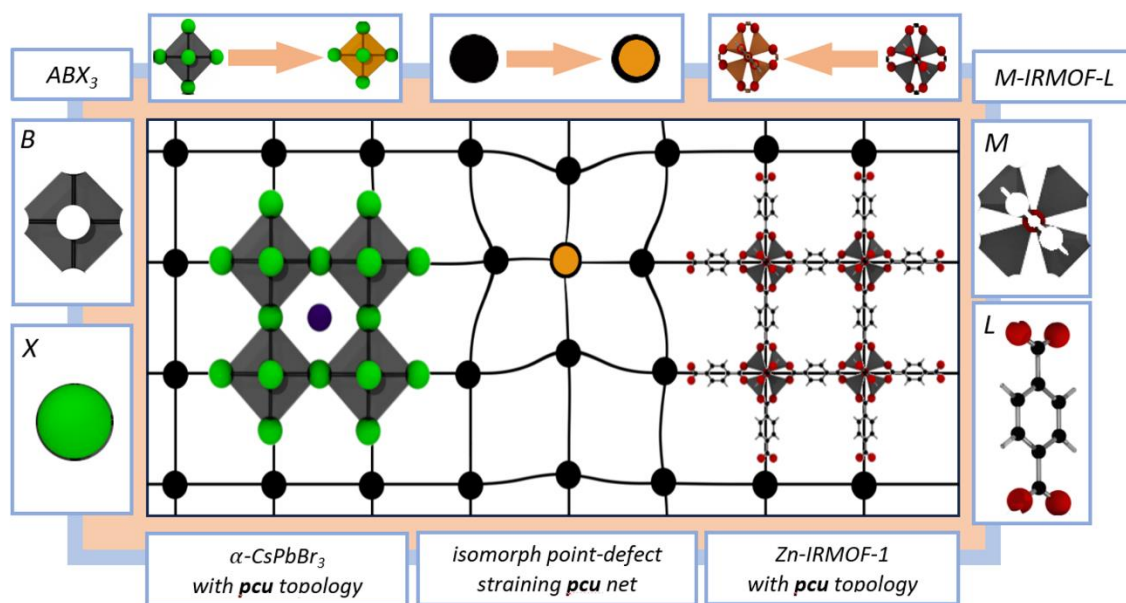
Designing the phase stability in metal-organic frameworks and metal halide perovskites: Two sides of the same strain coin?

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Disorder and strain introduced by dopants and defects have become increasingly essential to rationalise the design of nanostructured materials like metal-organic frameworks (MOFs) and metal halide perovskites (MHPs) [1], [2]. Strain engineering puts this strain at the heart of the design process by mapping the strained topology of the underlying net to its macroscopic properties, such as the material's phase stability [3]. Recently, we showed that such strain fields in MHPs are additive, and while their decay was fully correlated with the position of the strain-inducing defect within the lattice, it was found to be independent of its chemical nature [4]. This raises the question: can strain engineering constitute a material-transcending design tool unifying the impact disorder has in both MHPs and MOFs alike?

To explore this hypothesis, we herein trained *ab initio*-based machine learning potentials [5] to contrast point defects and their strain fields between two classes of MOFs and MHPs sharing the **pcu** topology: the M-IRMOF-L series [M={Zn, Be, Mg, Cd, Ca, Sr, Ba}, L={0-8, 10, 12, 14, 16, 18, 20}] and CsBX₃ perovskites [B={Ba, Pb, Ca, Mn, Zn, Ni}, X={Cl, Br, I}]. Besides investigating the generality of the strain decay rate within each material class, we compare how strain fields induced in one class inform the design of the other. To this end, we compare (i) strain fields induced by varying the metal ions in MOFs with those induced by changing B-site cation in perovskites and (ii) strain fields induced by changing the IRMOF linker with those induced by a change in the perovskite's X-site halogen. This, in turn, informs us of how we can impact the octahedral tilt and, hence, phase stability in MHPs and MOFs.



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References. [1] A. K. Cheetham, T.D. Bennett, F.-X. Coudert, A.L. Goodwin, *Dalton Trans.* **2016**, 45, 4113-4126. [2] J.A. Steele *et al.*, *J. Am. Chem. Soc.* **2021**, 143, 10500-10508. [3] S.M.J. Rogge, S. Borgmans, and V. Van Speybroeck, *Matter* **2023**, 6, 1435-1462. [4] J. L. Teunissen *et al.*, *J. Phys. Chem. C*, **2023**, 127, 23400-23411. [5] S. Vandenhoute *et al.*, *npj Comput Mater.* **2023**, 9, 19.