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Exploration of large *ab initio* data spaces to design structural materials with superior mechanical properties

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ABSTRACT

Modern engineering materials have evolved from simple single phase materials to nano-composites that employ dynamic mechanisms down to the atomistic scale. The structural and thermodynamic complexity of this new generation of structural materials presents a challenge to their design since experimental trial-and-error approaches as successfully used in the past are often no longer feasible.

Ab initio approaches provide perfect tools to new design routes but face serious challenges: Finite temperature free energies of the various phases are almost degenerate, requiring advanced theoretical formalisms that accurately capture all relevant entropic contributions.

In addition, their hierarchical nature with respect to length and time makes it challenging to explore the large range of chemical compositions. We have therefore developed a python based framework pyiron that allows in a highly automated way to combine accurate finite temperature first principles calculations with big data analytics.

The flexibility and the predictive power of these automated approaches will be discussed for examples ranging from the design of ductile Mg alloys, over describing the finite temperature behavior of high entropy alloys, to the discovery of general rules for interstitials in metals.

LOOKING FORWARD TO SEEING YOU!