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Ab initio guided design of structural materials with superior mechanical properties

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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 them challenging for any atomistic approach. Combining accurate first principles calculations with mesoscopic/macroscopic thermodynamic and/or kinetic concepts allows us now to address these issues and to determine free energies and derived thermodynamic quantities with a hitherto unprecedented accuracy. The flexibility and the predictive power of these approaches but also their present limitations will be discussed for examples ranging from modern ultra-high strength steels to light weight metallic alloys.