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Data, Disorder and Ceramics

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Abstract

Disordered multicomponent systems - occupying the mostly uncharted centers of phase diagrams - have been studied for the last two decades for their potential revolutionary properties. The search for new systems is mostly performed with trial-and-error techniques, as effective computational discovery is challenged by the immense number of configurations: the synthesizability of high-entropy ceramics is typically assessed using ideal entropy along with the formation enthalpies from density functional theory, with simplified descriptors or machine learning methods. With respect to vibrations — even if they may have significant impact on phase stability — their contributions are drastically approximated to reduce the high computational cost, or often avoided with the hope of them being negligible, due to the technical difficulties posed in calculating them for disordered systems. This is an area where data intensive techniques are making the difference and the presentation will illustrate some recent results.