INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

Monday, 19 February, 11:00 a.m.
Room IC 04-408

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The power of entropy in materials discovery

High-entropy materials have attracted considerable interest due to their combination of potentially unique properties and promising technological applications. Predicting their formation from previously known parameters remains the major hindrance to the discovery of new systems.

In this seminar, we introduce a descriptor - entropy forming ability - for predicting the synthesizability of such systems from first-principles calculations. The formalism, based on the energy distribution spectrum of randomized calculations, captures the accessibility of equally-sampled states near the ground state and quantifies configurational disorder potentially leading to high-entropy homogeneous single-phases. The methodology is used to seek for disordered refractory 5-metal carbides potential systems for ultra-high temperature applications. The descriptor correctly predicts a set of candidates that are experimentally synthesized as novel high-entropy homogeneous phases, validating the ansatz of the model. The method has the potential to accelerate the search and development of high-entropy crystalline systems by rationally combining first principles approaches with experimental synthesis.