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ABSTRACT:

Short-Range Order in Multi-Component Alloys with Ab Initio Trained Machine-Learning Potentials

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Short-range order (SRO) and its impact in compositionally complex materials has stimulated an intense debate within the materials science community. In contrast to long-range order, quantitative characterization of the nature and spatial extent of SRO evades most of the experimentally available techniques. Simulations at the atomistic scale have full access to SRO but face the challenge of accurately sampling high dimensional configuration spaces. In this talk I will discuss how recent advances in machine learning potentials allow to challenge the high dimensional phase space of compositionally complex alloys from ab initio. Examples include long- and short-range ordering in FCC CrCoNi alloys, refractory BCC NbMoTaW alloys as well as surface segregation in a CoCuFeMoNi alloy.