AI/ML for Scientific Discovery
Room Central Exhibit Hall - Session AIML-ThP

AI/ML for Scientific Discovery Poster Session

AIML-ThP-1 High-Throughput Ab Initio Screening of MAB Phases: Phase Stability and Mechanical Property Relationships, ***Nikola Koutna***, TU Wien, Austria; *L. Hultman,* Linköping Univ., IFM, Thin Film Physics Div., Sweden; *P. Mayrhofer,* TU Wien, Austria; *D. Sangiovanni,* Linköping Univ., IFM, Thin Film Physics Div., Sweden

MAB phases (MABs)—alternating atomically-thin ceramic and metallic-like layers—offer an interesting combination of mechanical, magnetocaloric, and catalytic properties, high-temperature oxidation resistance as well as damage tolerance, and have conquered a prominent role in the development of 2D materials. Despite their vast chemical and phase space, relatively few MABs have been achieved experimentally. In this poster I will present high-throughput ab initio screening of MABs that combine group 4–7 transition metals (M); Al, Si, Ga, Ge, or In (A); and boron (B). I will aim on revealing and understanding their phase stability trends and mechanical properties derived from elastic-constants-based descriptors. Considering the 1:1:1, 2:1:1, 2:1:2, 3:1:2, 3:1:3, and 3:1:4 M:A:B ratios and 10 competing phase prototypes for each elemental combination, the corresponding formation energy spectra of dynamically stable phases will be used to estimate the synthesisability of a single-phase MAB. Furthermore, the volumetric proximity of energetically-close MABs will allow identifying systems with possible transformation toughening abilities. The analysis of directional Cauchy pressures and Young's moduli will allow to analyze mechanical response parallel and normal to M–B/A layers. The poster will also suggest the most promising MAB candidates, including Nb_3AlB_4, Cr_2SiB_2, Mn_2SiB_2 or the already synthesised MoAlB.

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