



CRC Seminar Series

DATE: 14 October 2021
TIME: 3:00 PM – 5:00 PM
LOC: Online Zoom Meeting



GUEST SPEAKER:

Prof. Johanna Rosén

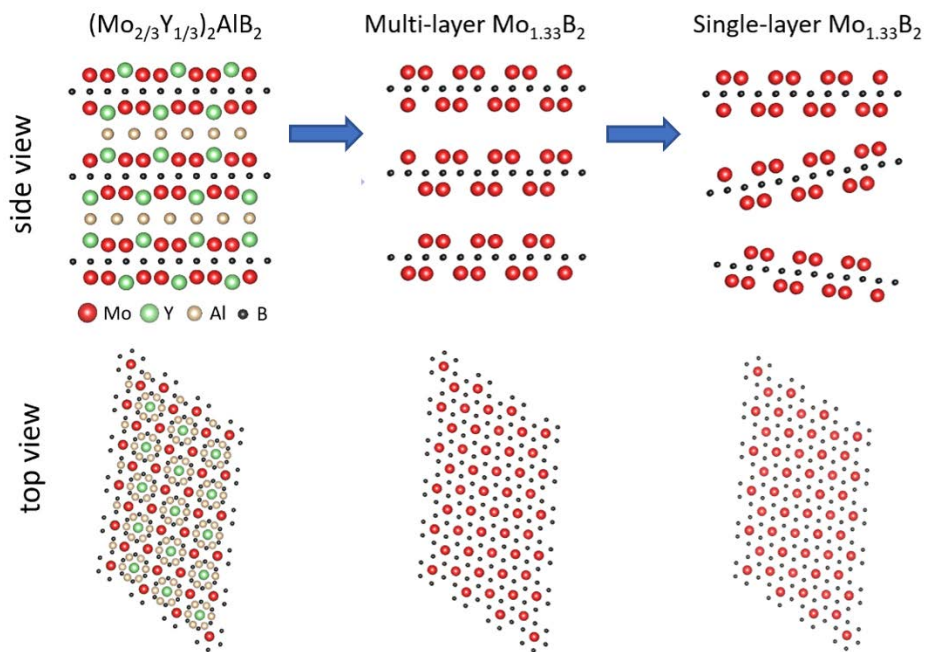
Linköping University, Materials Design

TITLE:

„New 3D and 2D Metal Borides from Materials Synthesis Guided by High-Throughput Simulations“

ABSTRACT:

The exploration of laminated metal carbides and nitrides in the form of MAX phases and MXenes is an area of materials discoveries. A more recent addition to the field is a new type of atomic laminated phases, coined *i*-MAX, in which the M-atoms in $(M_{1/3}M_{2/3})_2AlC$ are in-plane chemically ordered. The first phase discovered was $(Mo_{2/3}Sc_{1/3})_2AlC$, and it has been shown that this was a first example of a large, more than 30 reported to date, set of thermodynamically stable phases, typically obtained from an interplay between theoretical predictions and experimental verification. The *i*-MAX phases realize 3D and 2D materials with elements beyond those traditionally associated with MAX phases and MXenes, and expand the range of attainable properties. The present talk will summarise the current state of *i*-MAX and *i*-MXene synthesis, and how the knowledge and understanding of these materials can be transferred from atomically laminated carbides to corresponding borides. This has implications for the tuning potential in applications for, e.g., energy storage and catalysis. The 3D to 2D conversion of a laminated boride is shown in the image below.



PROFILE OF PROF JOHANNA ROSEN:

Professor Johanna Rosén is the Head of the Materials Design Division at the Department of Physics, Chemistry and Biology (IFM), at Linköping University in Sweden. She received her PhD from RWTH-Aachen University in Germany, and after being a post doc and visiting scientist at LBNL in Berkeley (USA) and at Sydney University (Australia), she returned to Sweden to establish her research platform. Her research interest is theoretical and experimental studies targeting novel 3D and 2D materials, including carbides (MXenes), oxides and borides, for studying, e.g., magnetism and energy storage. Johanna is since 2012 a Wallenberg Academy Fellow, and since 2017 a member of the Young Academy of Sweden.