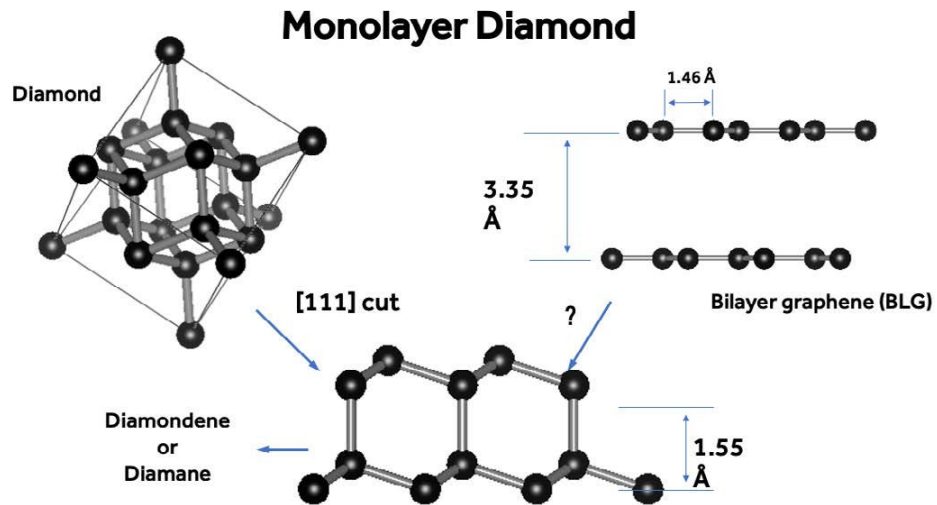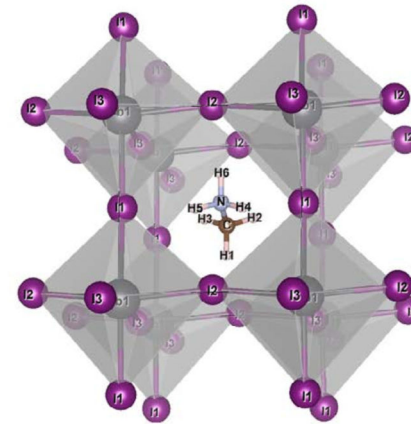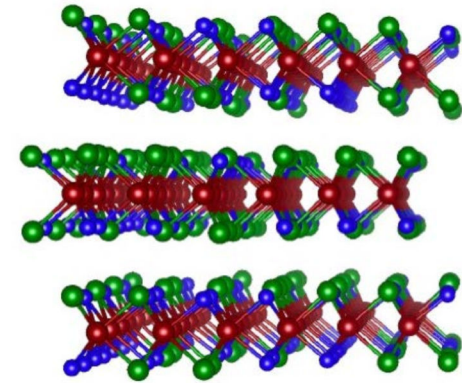# COMPUTATIONAL MATERIALS, DATA SCIENCE & SIMULATION
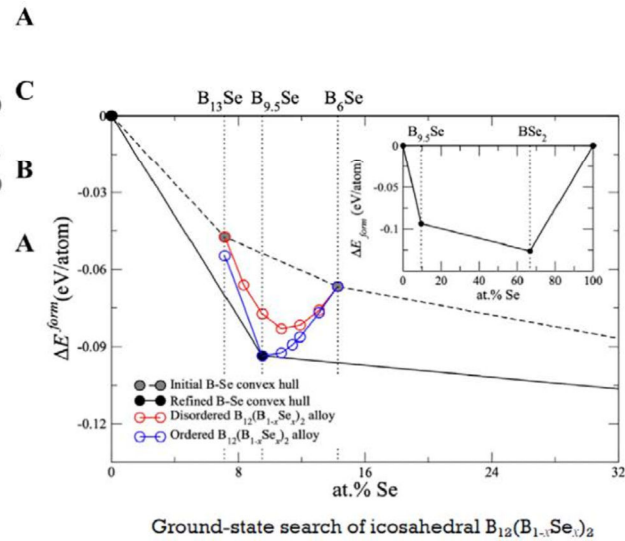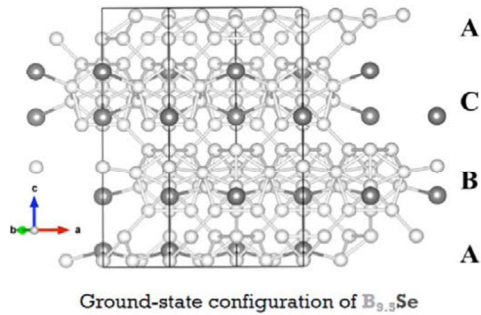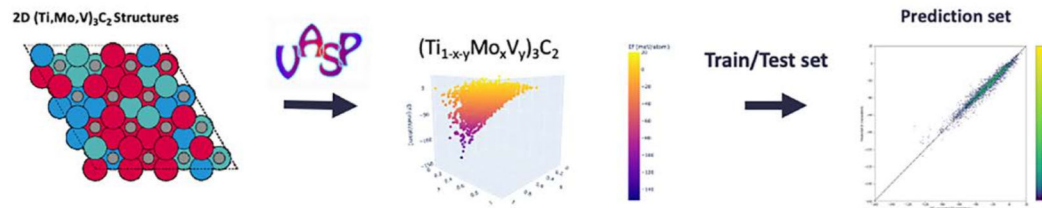
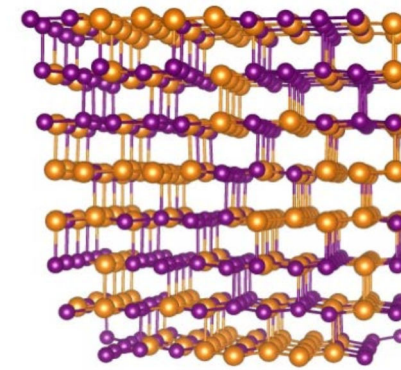## Monolayer Diamond

Hybrid-Perovskite Structure for Solar Cell Application

COMPUTATIONAL MATERIALS, DATA SCIENCE & SIMULATION

Simulation of thermodynamic stable phases of multi-transition metal MXenes

2D (Ti,Mo,V)$_3$C$_2$ Structures

$(Ti_{1-x-y}Mo_xV_y)_3C_2$

Train/Test set

Prediction set

Ground-state configuration of $B_{9.5}$Se

B_{13}Se $B_{9.5}$Se B_6Se

$B_{9.5}$Se BSe_2

ΔE^{form} (eV/atom)

at.% Se

- Initial B-Se convex hull
- Refined B-Se convex hull
- Disordered $B_{12}(B_{1-x}Se_x)_2$ alloy
- Ordered $B_{12}(B_{1-x}Se_x)_2$ alloy

Ground-state search of icosahedral $B_{12}(B_{1-x}Se_x)_2$

Visualization of $2H$-$W(Se_{0.5}Te_{0.5})_2$ random solid solution

$Bi_{0.5}Sb_{0.5}$ random solid solution

i-SMaT