Design Guidelines for Two-Dimensional Transition Metal Dichalcogenide Alloys

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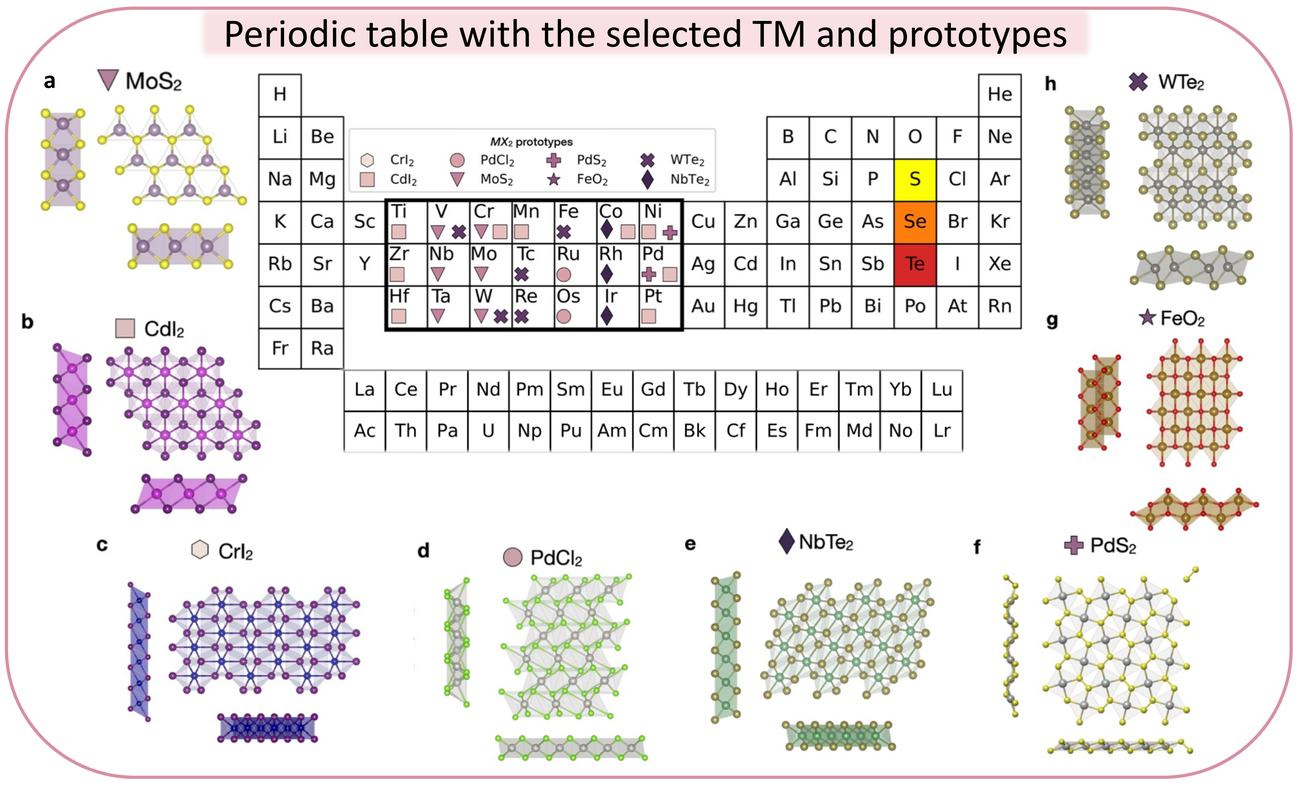
Background

- 2D materials and TMDs in particular are at the forefront of nanotechnology.
- How to comprehensively explore 2D ternaries and binary alloys of TMDs?

Method

- Ab Initio Calculations
- Cluster Expansion model training
- Approximated Boltzmann Sampling

Periodic table with the selected TM and prototypes



Our contributions

We present a Pettifor map where the 2D TMDs can be consulted. With this map, we can explore the thermodynamic phase behavior, ternaries and binary alloys of TMDs.

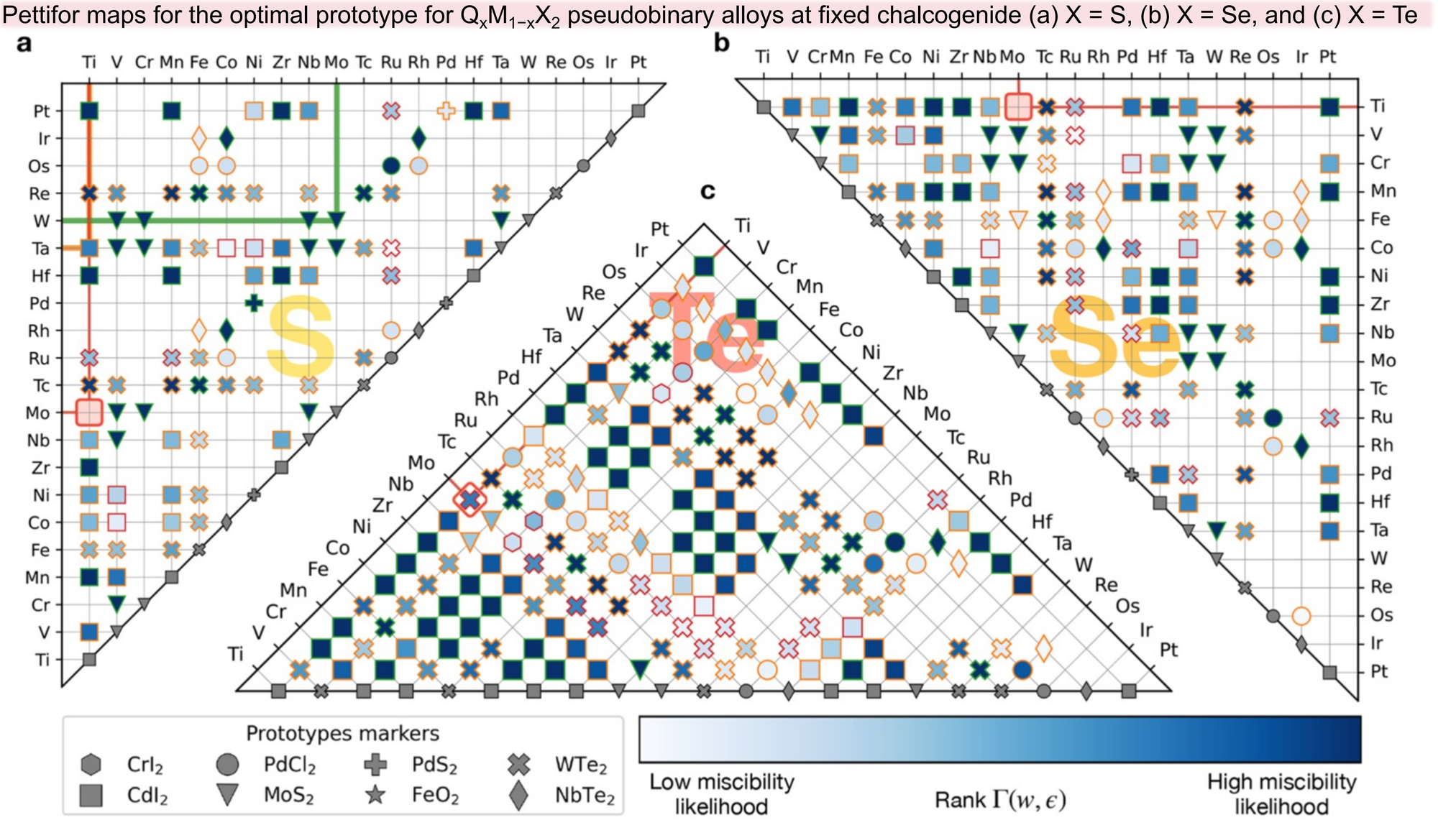
Applications

- Nanoscale eigineering applications
- 2D materials for technological applications
- guideline for synthesis of TMDs binary alloys

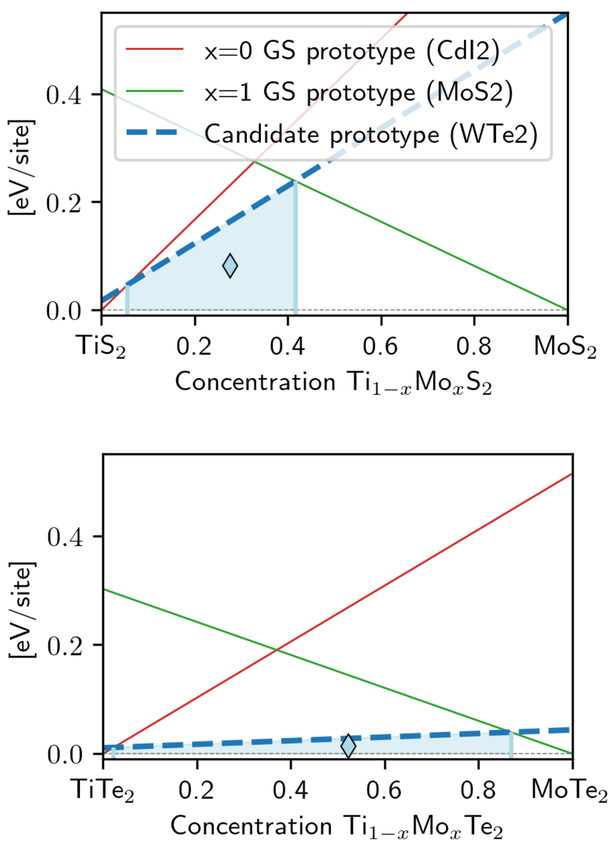
Computational results

1. Pettifor maps

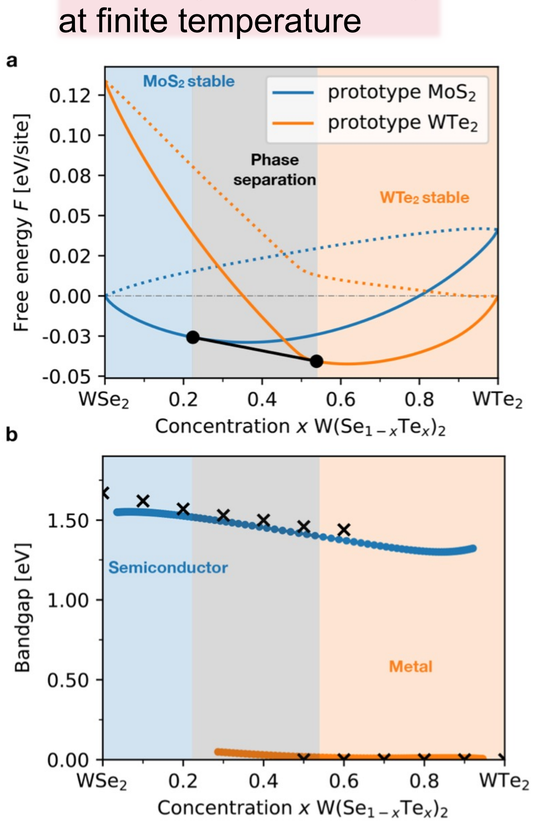
Pettifor maps for the optimal prototype for $Q_xM_{1-x}X_2$ pseudobinary alloys at fixed chalcogenide (a) X = S, (b) X = Se, and (c) X = Te



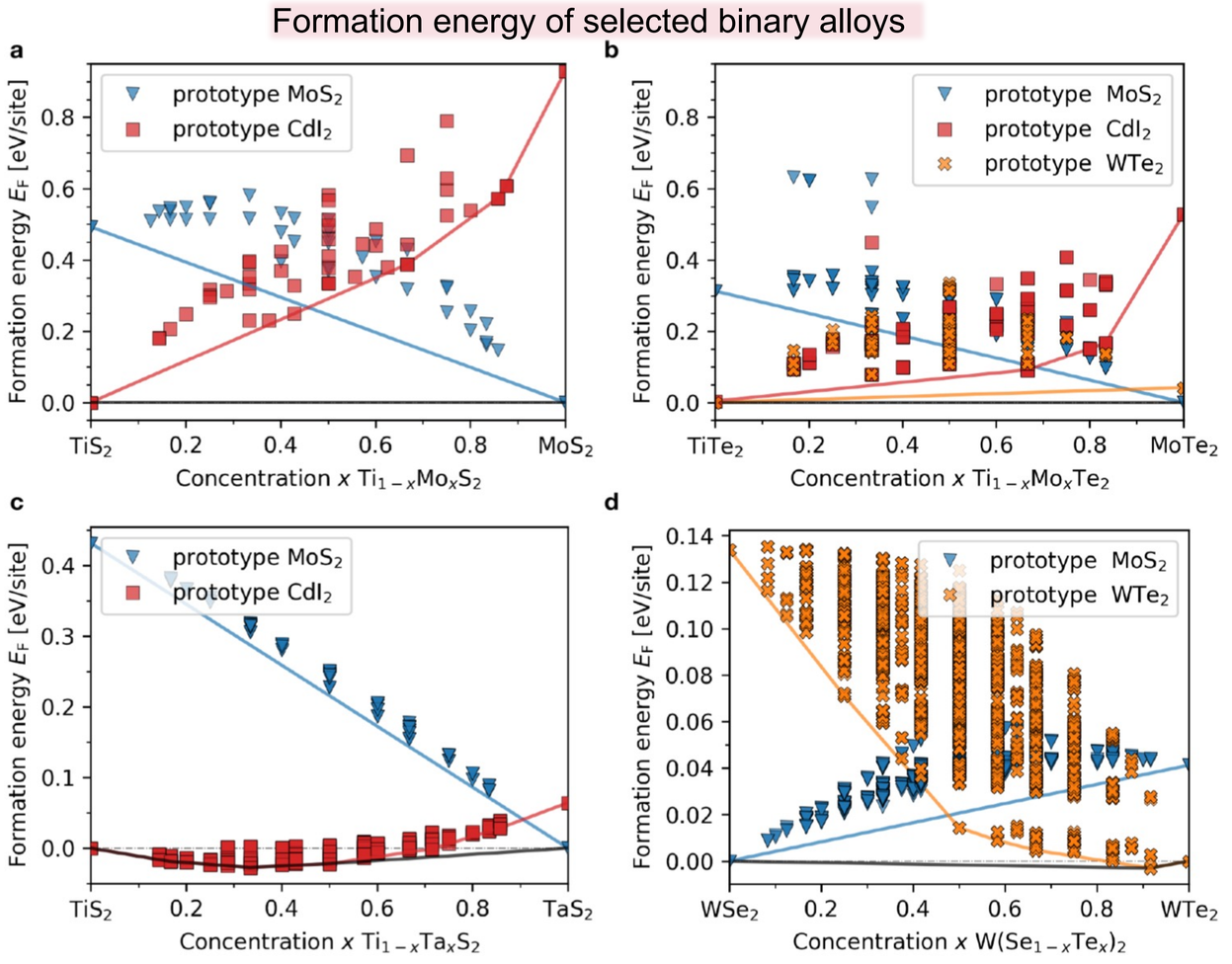
Examples of metastability metric



Thermodynamic stability at finite temperature



Formation energy of selected binary alloys



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Publications:

[1] A. Silva, J. Cao, T. Polcar and D. Kramer, Chem Mater 34, 10279 (2022).
[2] A. Silva, J. Cao, T. Polcar and D. Kramer, npj Comput Mater 8, 178 (2022).
[3] A. Silva, T. Polcar, and D. Kramer, Comput Mater Sci 186, 110044 (2021).

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