Session of "Fokus Materialchemie" – Wednesday, **08.10.2025** 14:00
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Data-Driven Prediction of Interface Stability

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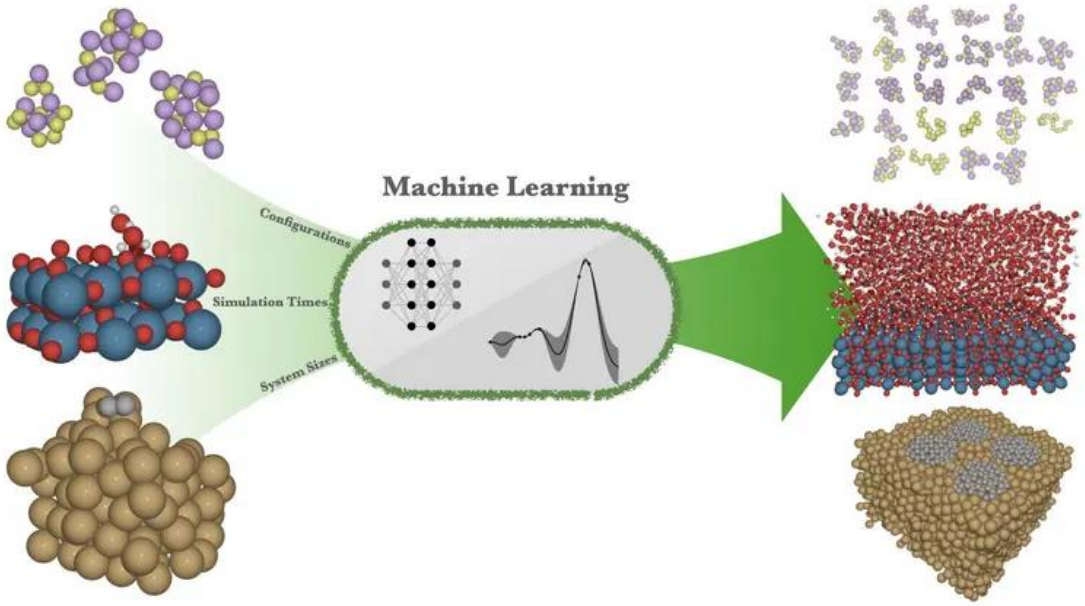
Predicting the stability of interfaces is a key challenge in materials design, as their atomic configuration strongly influences device performance. Traditionally, density functional theory (DFT) serves as the standard approach for assessing interface stability. However, due to the large configurational space arising from multiple possible terminations and crystallographic orientations, exhaustive DFT calculations quickly become computationally infeasible.

In this work, I developed a data-driven pipeline for efficient interface stability prediction. The workflow integrates data retrieval from the Materials Project database, automated interface construction using *pymatgen*, and stability evaluation employing machine learning interatomic potentials based on MACE Foundation Models. Three independent stability criteria were implemented to assess interface energetics.

The pipeline was validated for the Ti_3SiC_2 (MAX phase) / 4H-SiC system, a material combination relevant to Infineon Technologies. Remarkably, the experimentally observed most stable configuration (001/001 interface) was consistently reproduced across all stability criteria. This suggests that MACE models—although trained solely on bulk structures—are capable of capturing the energy trends of slabs and interfaces as well. The developed approach will be integrated into Infineon's broader materials discovery workflow for targeted device optimization.



Bridging classical atomistic simulations and large-scale modeling through MLIPs [1].

References

[1] Heenen Group, Fritz Haber Institute of the Max Planck Society. https://www.fhi.mpg.de/739215/heenen_group, accessed October 2025.