IAP Seminar

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Tuesday, 29th November 2022, 16:00 s.t.
TU Wien, Institut für Angewandte Physik, E134
1040 Wien, Wiedner Hauptstraße 8-10
Yellow Tower „B“, 5th floor, SEM.R. DB gelb 05 B

The seminar will be also held as a Zoom Meeting
https://tuwien.zoom.us/j/93979999148?pwd=Q3ZsMXJFVzB3QjBnKzRaZHV6MWNzZz09
ID meeting: 939 7999 9148
Passcode: nzGD3M0B

Machine Learning backed Evolutionary Search: Atomic Structure in Surface Reconstructions

Atomic structure determination of surface reconstructions has typically relied on structural models derived from intuition and domain knowledge. While evolutionarystrategies combined with first-principles computations based on density functional theory have proven powerful tools for structure searches, the computational cost is prohibitive, even on modern hardware. We facilitate the thorough exploration of potential energy landscapes at reasonable cost by combining the efficient covariance matrix adaptation evolution strategy (CMA-ES) with a neural-network force field (NNFF) utilizing Google JAX with just-in-time compilation and end-to-end automatic differentiation.
The first part of the presentation will cover the methodology used for exploring $SrTiO_3$ (110) n°ø 1 overlayer structures and discuss the transferability of the NNFF and the results that were obtained, including known and new low-energy reconstructions. Building on this, an active learning approach that will allow us to investigate more complicated structures, e.g., $SrTiO_3$ (110) 2°ø n surfaces, will be outlined. Finally, an outlook on planned applications of the presented methodology will be given.

All interested colleagues are welcome to this seminar lecture
(45 min. presentation followed by discussion).

Friedrich Aumayr
(LVA-Leiter)

Michele Riva
(Seminar Chair)