7th live session of **Focus Materialchemie** – Wednesday, **14.06.2023** 16:00 – @ **Seminarraum Lehar 01** (TU-Wien, Getreidemarkt 9, BC, OG. 01, room A46) – join us on **ZOOM** (ID: 983 0066 2349)

Accelerated Search for Surface Reconstructions Through Chemical and Structural Space

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To determine the atomic structure of surface reconstructions, structural models derived from domain knowledge and intuition have historically been essential. Evolutionary algorithms combined with density functional theory have proven to be powerful tools for such structure searches if one accepts the prohibitive cost that comes with a thorough exploration of a potential energy surface. We utilize state-of-the-art machine learning methods to significantly reduce computational cost and gain access to more complex structures without sacrificing accuracy.