Machine Learning for Materials Hard and Soft
ESI-DCAFM-TACO-VDSP Summer School 2022
11–22 July 2022
ESI, University of Vienna

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Machine learning-enabled enhanced sampling and ultra-fast molecular simulators

Abstract:
Data-driven modeling and deep learning present powerful tools that are opening up new paradigms and opportunities in the understanding, discovery, and design of soft and biological materials. First, I will describe our use of autoencoding neural networks to learn data-driven collective variables in molecular systems and drive enhanced sampling within interleaved rounds of variable discovery and biased calculations. Second, I will describe an approach based on latent space simulators to learn ultra-fast surrogate models of molecular systems by stacking three specialized deep learning networks to (i) encode a molecular system into a slow latent space, (ii) propagate dynamics in this latent space, and (iii) generatively decode a synthetic molecular trajectory.