Understanding trajectories: From electron microscopes to atomistic simulations

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With the development and availability of more computational capabilities including accessible CPU/GPUs, efficient algorithms, and corresponding implementations, there has been significant advancements in the field of physical simulations at different length scales, in the past couple of decades. The electron and scanning probe microscopies have also emerged as keystone tools for the exploration of matter on the atomic and mesoscale levels. However, utilization of theoretical models to guide, perform experiments and refine the parameters in both spaces, to establish a continuous feedback-loop, are still at an early stage. Subsequently, there is a need to bridge this gap to allow for co-navigation of theory and experiment to develop comprehensive physics of materials. This talk will focus on examples of such open-source workflows aiming at establishing a bridge environment between the instrument-specific libraries and general physical analysis. These enable seamless deployment of several deep learning algorithms on-the-fly for appropriate feature finding, property predictions in combination with atomistic simulations to explore underpinning causal mechanisms. Initially constructed and implemented on graphene like 2D systems, these frameworks perform remarkably well, when extended to protein nanorods. Discussion on studies with physics-augmented probabilistic models, along with simulations-imaging driven reinforcement learning strategies will be included in the presentation.

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