Towards Differentiable, Machine-Learning-Accelerated Battery Simulations Across Scales

Associate Professor Arghya Bhowmik[1]
[1]Technical University Of Denmark, , Denmark

Battery behavior emerges from tightly coupled phenomena spanning electronic, atomic, mesoscopic, and cell-level scales, yet these regimes are still largely modeled in isolation. In this talk, I will present a vision for machine-learning-accelerated simulation frameworks that not only speed up models across scales, but also render them differentiable and composable as a single end-to-end object for cross-scale optimization. I will discuss our progress in building surrogate and generative models for electronic-structure and atomistic simulations, as well as recent efforts to accelerate or replace phase-field models at the mesoscale and multiphysics cell-level models at the macroscale. Together, these developments point toward a new paradigm for batteries: differentiable multiscale simulation pipelines that enable rapid design, inverse modeling, and optimization across the full hierarchy of battery physics.