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How to Use Workflow Frameworks to Simulate Charge Transport in Organic Electronics

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Abstract:

The goal of this tutorial is to realize the concept of workflows in practice on the example of a simple multiscale model for charge transport in organic electronics. The model will include morphology generation, selecting charge-transfer sites, parallel computations of the parameters for Marcus rate expression, and calculation of charge mobility. Using two different workflow modeling frameworks, UNICORE (https://www.unicore.eu/) in the first session and FireWorks (https://pythonhosted.org/FireWorks/) in the second session, the participants will learn how to construct a workflow and how to setup and perform a workflow simulation. Computational aspects such as concurrency, efficiency, and different dataflow realizations will be especially emphasized. In addition, the Atomic Simulation Environment (ASE) will be introduced as a tool for simulation code abstraction and integration. Based on ASE, participants will learn how to replace, for example, one code for electronic structure calculation with another without having to change their model.