

Lecturer: F. Evers:

Topic: Transport from ab-initio

The lecture offers a concise and pedagogical introduction into the theory of ab-initio based transport calculations. Specifically, the following topics will be covered:

- transport formalism: Landauer Büttiker theory
- ab-initio theories: DFT: basic theory and Kohn-Sham formulation
- transport implementations with finite-size Hilbert spaces
- inelastic features, coupling to mechanical degrees of freedom
- fundamental aspects of the approach and its limitations

