Concepts in Electrocatalysis
preliminary list of content

The electrical double layer

- Gouy-Chapman-Stern model
- metal / electrolyte interface: contribution of the metal, jellium and results from DFT
- semiconductor / electrolyte interface: space charge in the semiconductor
- special cases: graphite electrodes, carbon nanotubes
- space charge in the solution: hard sphere model and extensions, results from computer simulations

A few thermodynamic concepts

- chemical and electrochemical potential
- electrode potential on the vacuum scale
- surface tension and surface stress

Reaction rates in condensed phases

- fluctuations and random motion: Langevin equation
- Kramer's theory
- Comparison with Eyring's theory

Electronic structures of solids

- free electron model
- band formation in solids
  - Bloch's theorem
  - tight binding model (onde-dimensional)
  - Kronig-Penney model

Fundamental concepts for electron transfer in condensed phases

- solvent reorganization
- adiabatic and non-adiabatic transitions

Classical theories of electron transfer

- theories of Marcus and Hush
- application to electrochemical systems
- formulation of Gerischer

Quantum theories of electron transfer

- Hamiltonian for electrochemical electron transfer
- weak interactions: Levich-Dogonadze theory
- adiabatic reactions

Band effects on electron transfer

- Anderson-Newns theory
- wide band approximation
- interaction with a narrow band
- Nørskov d-band model

Electrocatalysis in Santos-Schmickler theory

- combination of DFT with model Hamiltonian
- solvent reorganization and potential of mean forces
- reaction free-energy surfaces

Special cases

- hydrogen electrocatalysis – beyond the volcano plot
- the enigma of metal deposition
- oxygen reduction in alkaline solutions

Nanostructured electrodes
possible topics: steps, metal clusters, various forms of carbon electrodes.