Freie Universität Berlin

Institute of Chemistry and Biochemistry

Course description

Course Title Statistical Thermodynamics Termodinâmica Estatística		
Type/Attendance Time Lecture: 2 hour per week Tutorial: 2 hours per week	**Credit points (ECTS)** 5	**Type of Examination** Examination, Exercises
Recommended Prerequisites [entrance requirements to be entered]		

Content

1. Mathematical Fundamentals

Probability theory, distribution functions, mathematical tools (e.g. Stirling approximation for factorials, Lagrangian methods for Extrema subject to boundary conditions)

2. Physical and quantum mechanical fundamentals

Phase space, Ergodic hypothesis, description of quantum and classical mechanics, model systems for molecular motion: free particle, particle in a box, oscillator, rotator, spin and nuclear spin (fermions and bosons)

3. Microcanonical and canonical ensembles (in perspective with the grand canonical ensemble)

Occupancy of phase space, composition of phase space, micro and macro conditions, thermodynamic equilibrium, Boltzmann statistics, temperature, microscopic definition of macroscopic state functions: internal energy and entropy statistical thermodynamic formulation of the three laws of thermodynamics, non-adiabatic and adiabatic processes.
Outlook on non-equilibrium distributions (e.g: population inversion)

4. Partition functions and thermodynamic functions

Partition functions of translation, vibration, rotation, molecular and system partition functions for discriminable and non-discriminable particles, the relation of partition functions to thermodynamic functions and equilibrium constants, partition functions for the statistical description of reactive scattering (Eyring's transition state theory)

5. Quantum statistical thermodynamics for fermions and bosons

Fermi-Dirac distribution of fermions, Bose-Einstein distribution of bosons

Conteúdo

1. Fundamentos matemáticos;
2. Fundamentos físicos e da mecânica-quântica;
3. Conjuntos microcanônicos e canônicos ;
4. Funções de partição e funções termodinâmicas;
5. Termodinâmicas quântica-estatística para férmions e bósons.