

C7790 Introduction to Molecular Modelling

TSM Modelling Molecular Structures

Lesson 3 Intermezzo I

PS/2021 Present Form of Teaching: Rev2

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Overview

macroworld

microworld

states

(thermodynamic properties, G , T ,...)

phenomenological thermodynamics

equilibrium (equilibrium constant)

kinetics (rate constant)

free energy
(Gibbs/Helmholtz)



partition function

statistical thermodynamics

microstates

(mechanical properties, E)

microstate \neq microworld

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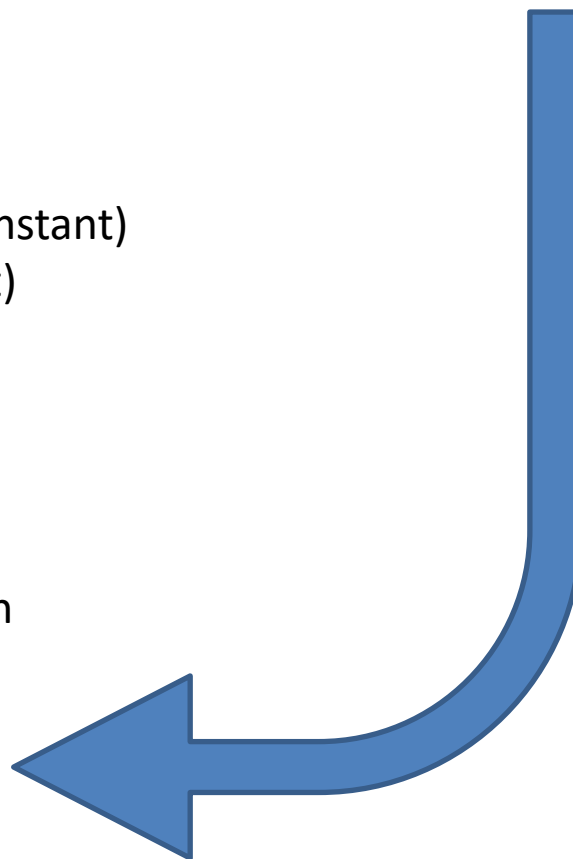


partition function

statistical thermodynamics

microstates

(mechanical properties, E)



physical description

microstate \neq microworld

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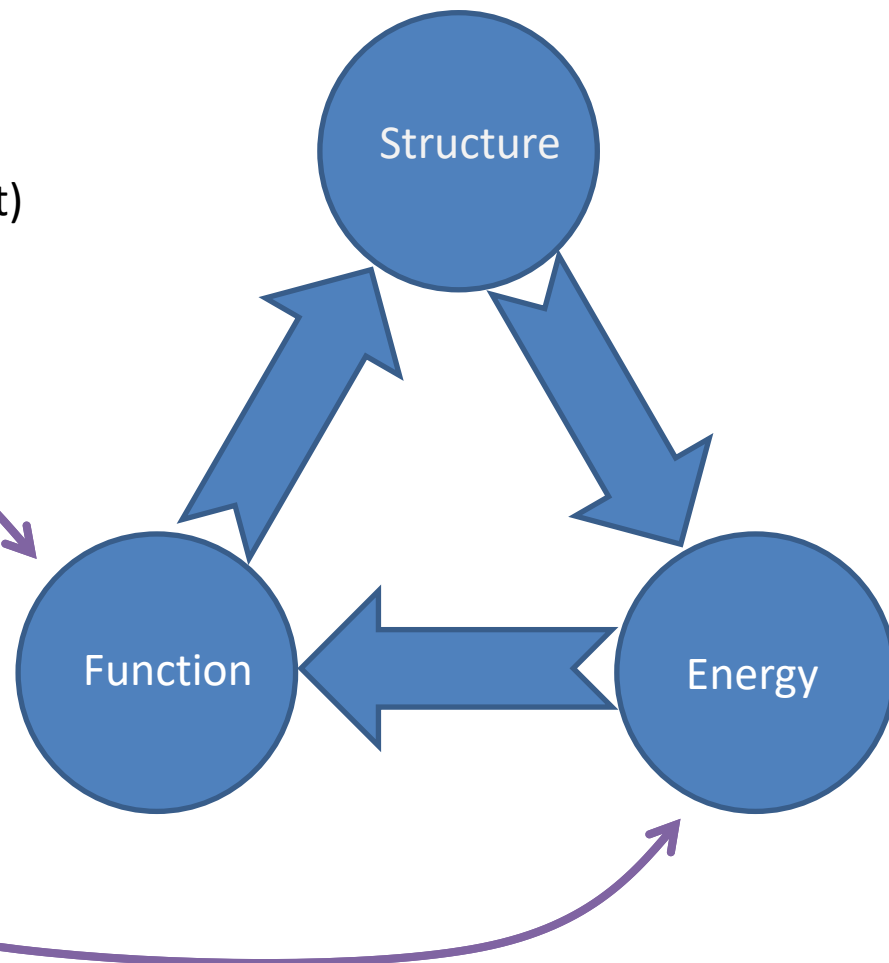
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Description levels (model chemistry):

- quantum mechanics
 - semiempirical methods
 - ab initio methods
 - post-HF methods
 - DFT methods
- molecular mechanics
- coarse-grained mechanics

Simulations:

- molecular dynamics
- Monte Carlo simulations
- docking
- ...

