Chemical dynamics & molecular interaction

overall goal: micro to macro

molecular structure

quantum mechanics

molecular interactions

quantum mechanics

molecular dynamics

sampling

configuration space

partition functions

statistical thermodynamics

free energy

thermodynamics

molecule-free

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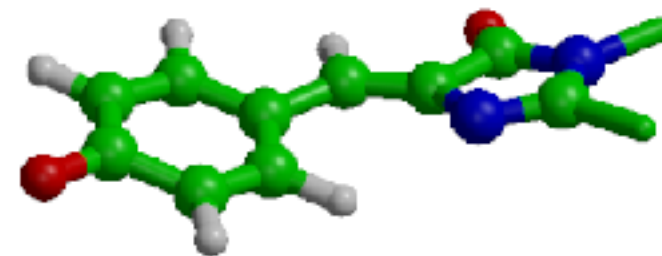
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molecular dynamics

sampling

configuration space
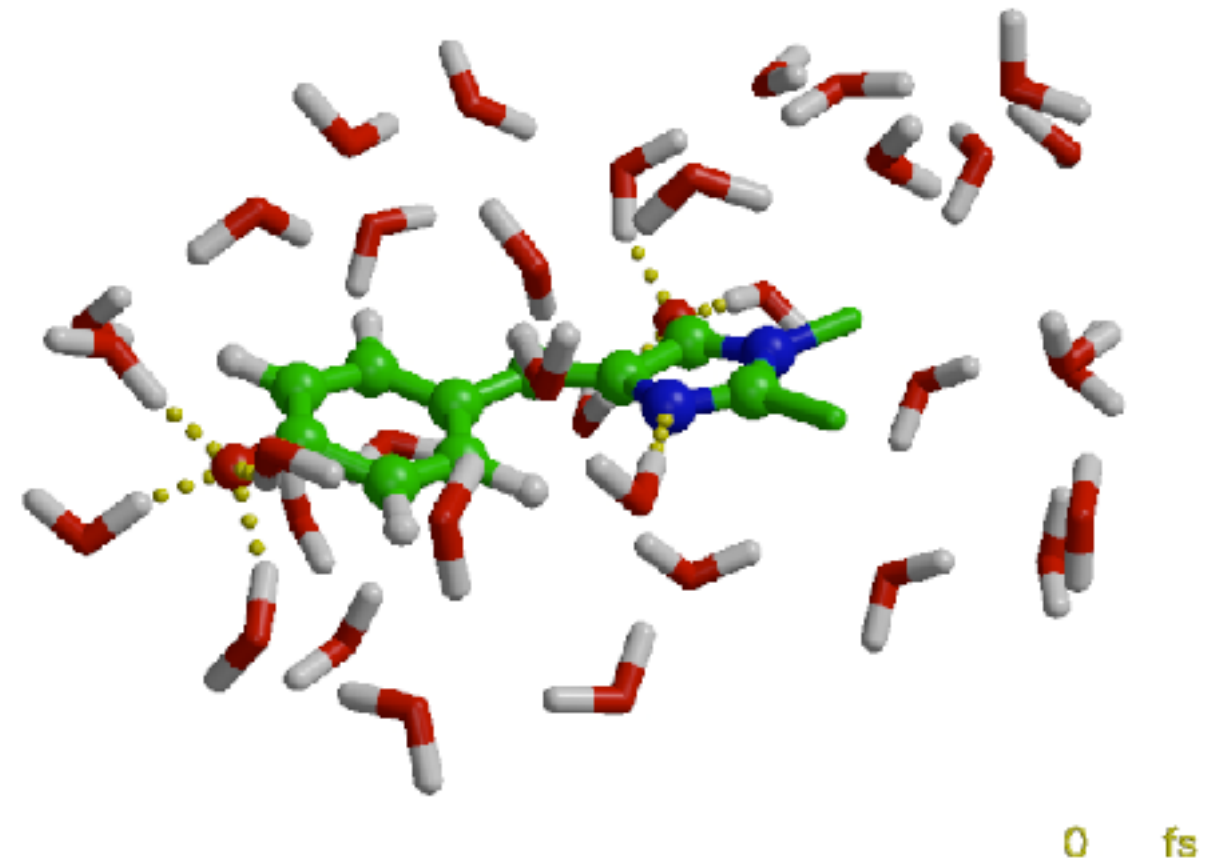
partition functions

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0   fs

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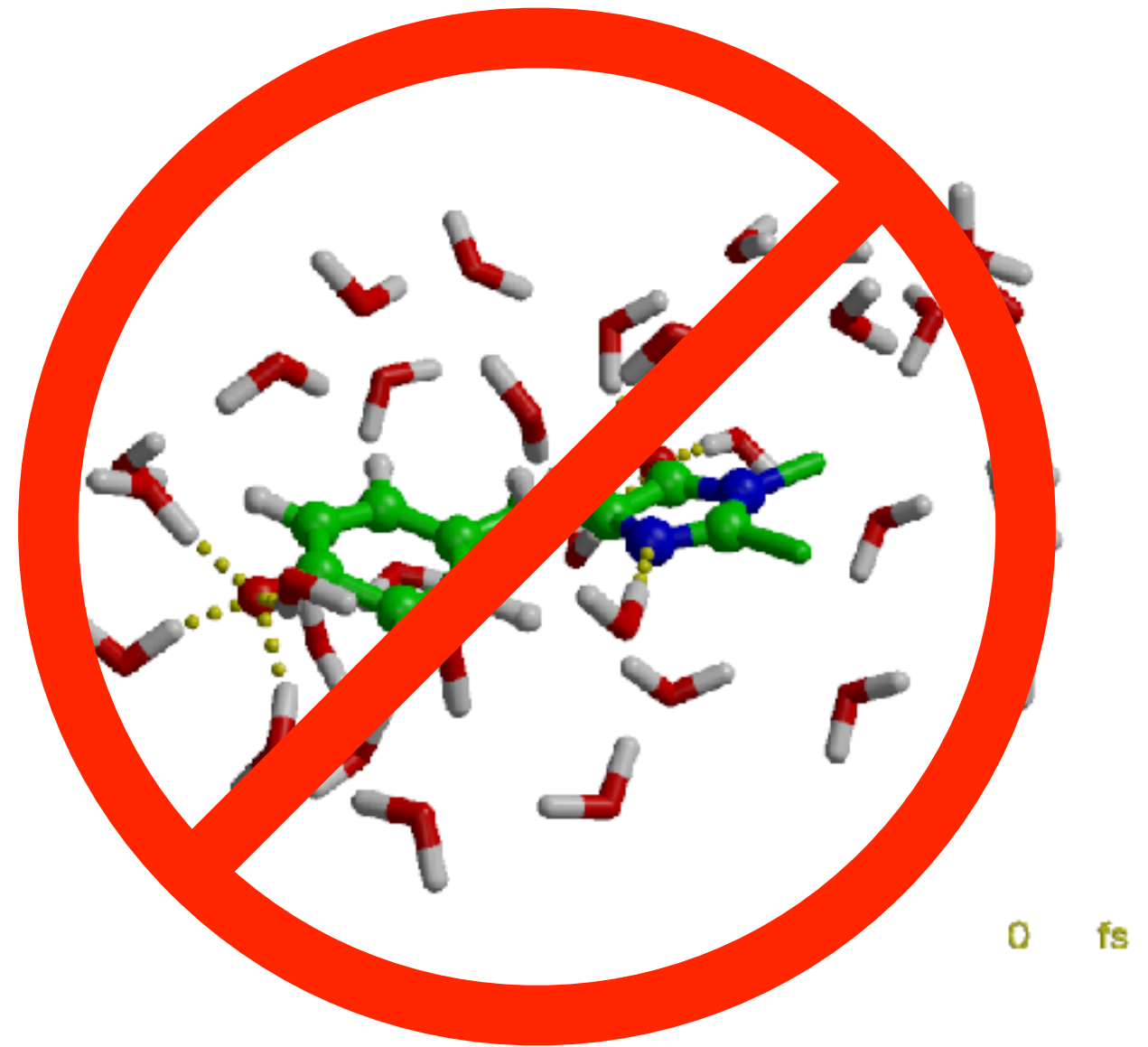
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0   fs

Chemical dynamics & molecular interaction

two options

basic: 3 credits

lectures

homework exercises

exam

advanced: 3 additional credits

project

written report

oral presentation

Chemical dynamics & molecular interaction

content (could be changed still)

1 thermodynamics refresher

equation of state of ideal gas

first & second laws of thermodynamics

Carnot engine

'discovery' of entropy

demonstration (maybe)

efficiency of steam engine

molecule-free

Chemical dynamics & molecular interaction

content (could be changed still)

2 statistical mechanics/thermodynamics

from micro (molecules) to macro (bulk)

micro state

macro sate

statistical weight

Boltzman definition of entropy

partition function

free energy

ensembles

micro-canonical

canonical

grand-canonical

Chemical dynamics & molecular interaction

content (could be changed still)

3. molecular interactions

   intramolecular interactions

   intermolecular interactions

   electrostatic

   dispersion

   hydrogen bonds

   evaluating intermolecular interactions

   Ewald summation: energy of crystal

   partition function

   classical statistics

   phase space

Chemical dynamics & molecular interaction

content (could be changed still)

4. chemistry

equilibrium

free energy

equilibrium constant

rates

reaction coordinates

Arrhenius' law

Eyring's transition state theory

Krames' theory

Chemical dynamics & molecular interaction

content (could be changed still)

5. difficult stuff

quantum statistics

black body radiation

hydrophobic effect

self-aggregation

fluctuations & non-equilibrium processes

jarzynski/Crooks theorema

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