More quantum chemistry with BOINC

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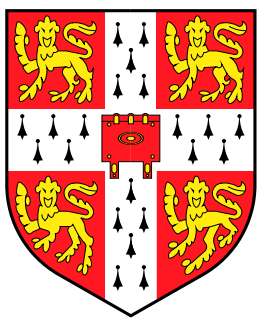
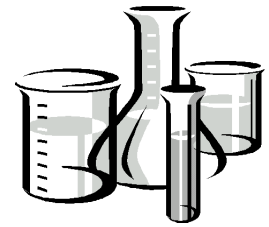


From Chemistry to Quantum Chemistry

Chemistry

- science of composition, properties and changes of matter
- organic (carbon-based) chemistry, biochemistry, ...



Theoretical chemistry

- use of reasoning and computation to predict chemical phenomena
- chemoinformatics, molecular modeling, ...

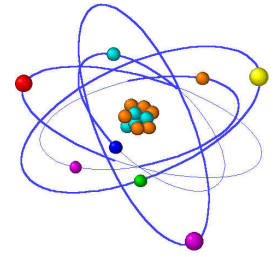
Quantum Chemistry

- applies quantum mechanics to address problems in chemistry
- prediction of structure and reactivity of atoms and molecules

Quantum Chemistry

Molecular electronic structure theory

- mathematical description of matter at the molecular scale
- based on the (electronic) Schrödinger equation

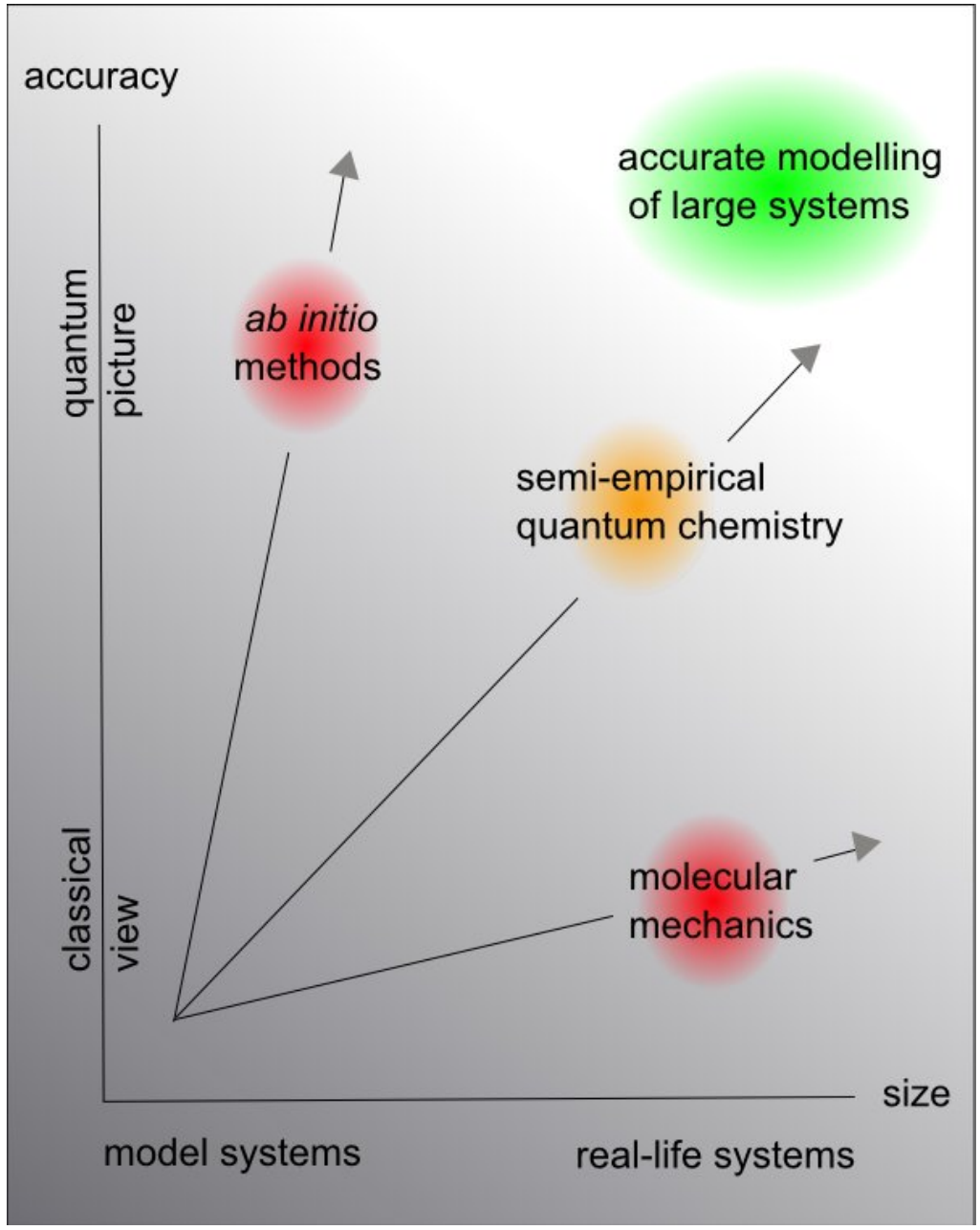


Hierarchy of general approximations

- pure 'ab initio' quantum mechanical treatment like DFT (QM)
- semiempirical QM treatments like AM1 (SE)
- (classical molecular mechanics treatments like AMBER (MM))

Hierarchy of QM approximations

- Hartree-Fock, post-Hartree Fock methods like MP2
- Density Functional Theory, Jacob's ladder of approximations


accuracy
quantum picture
classical view
accurate modelling of large systems
ab initio methods
semi-empirical quantum chemistry
molecular mechanics
size
model systems
real-life systems

Accurate modeling of large systems?

The hybrid QM/MM ansatz

- important inner region is described on QM level
- large outer region described on MM level
- approaches differ in how they combine both descriptions

Existing QM/MM approaches

- based on standard QM (DFT) and MM (force fields) methods
- already very successful in describing the reactivity of biomolecular systems e.g. enzyme catalysis, photosynthesis, ...

Our QM approach: Fixed Node Diffusion Monte Carlo

What?

- models the electronic Schrödinger equation ...

$$\frac{\partial \Psi(r,\tau)}{\partial \tau} = \frac{1}{2m}\nabla^2\Psi(r,\tau) - V(r)\Psi(r,\tau)$$

- ... as a generalized diffusion process

$$\frac{\partial c(r,t)}{\partial t} = D\nabla^2 c(r,t) - k(r)c(r,t)$$

Why?

- exact solution within the so-called 'fixed node' approximation
- very well suited for parallelization

Our project: Quantum Monte Carlo at home

Already enabled us to find out ...

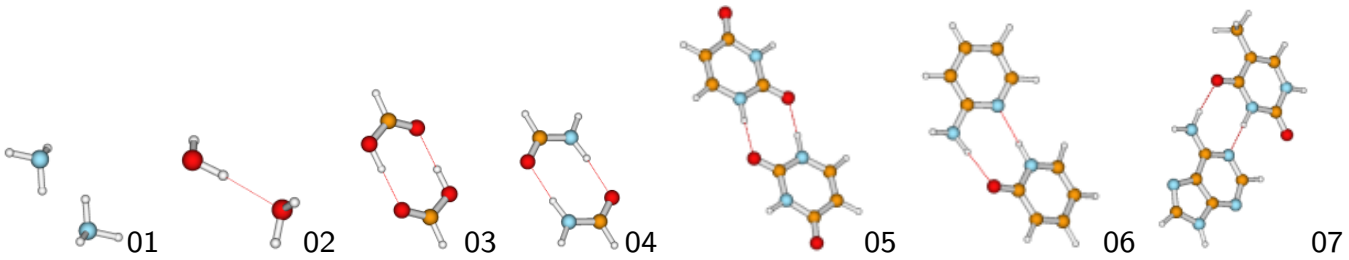
- ... how to do accurate and reliable FNDMC calculations for important biomolecular model systems like DNA base pairs
- ... how much effort is needed to keep the effects of the 'fixed node' approximation small for the calculation of reaction energies

And will now move on to ...

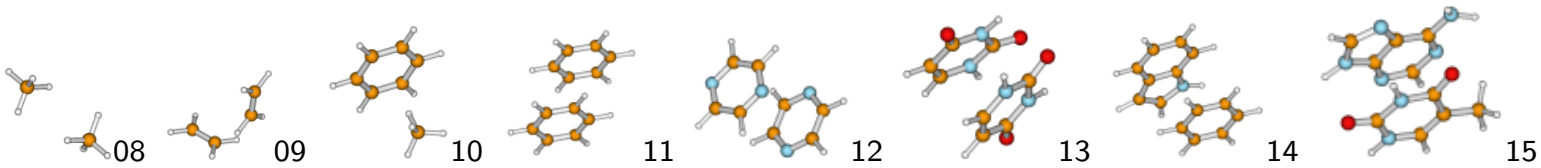
- ... develop a QM/MM scheme with FNDMC to treat larger QM regions with higher accuracy
- ... calculate reference data for biomolecular systems with relevance in enzyme catalysis

biomolecular model systems

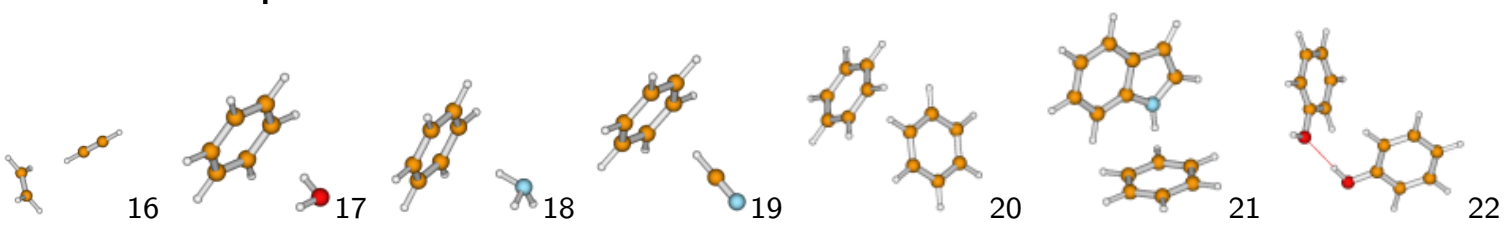
Hydrogen-bond dominated:



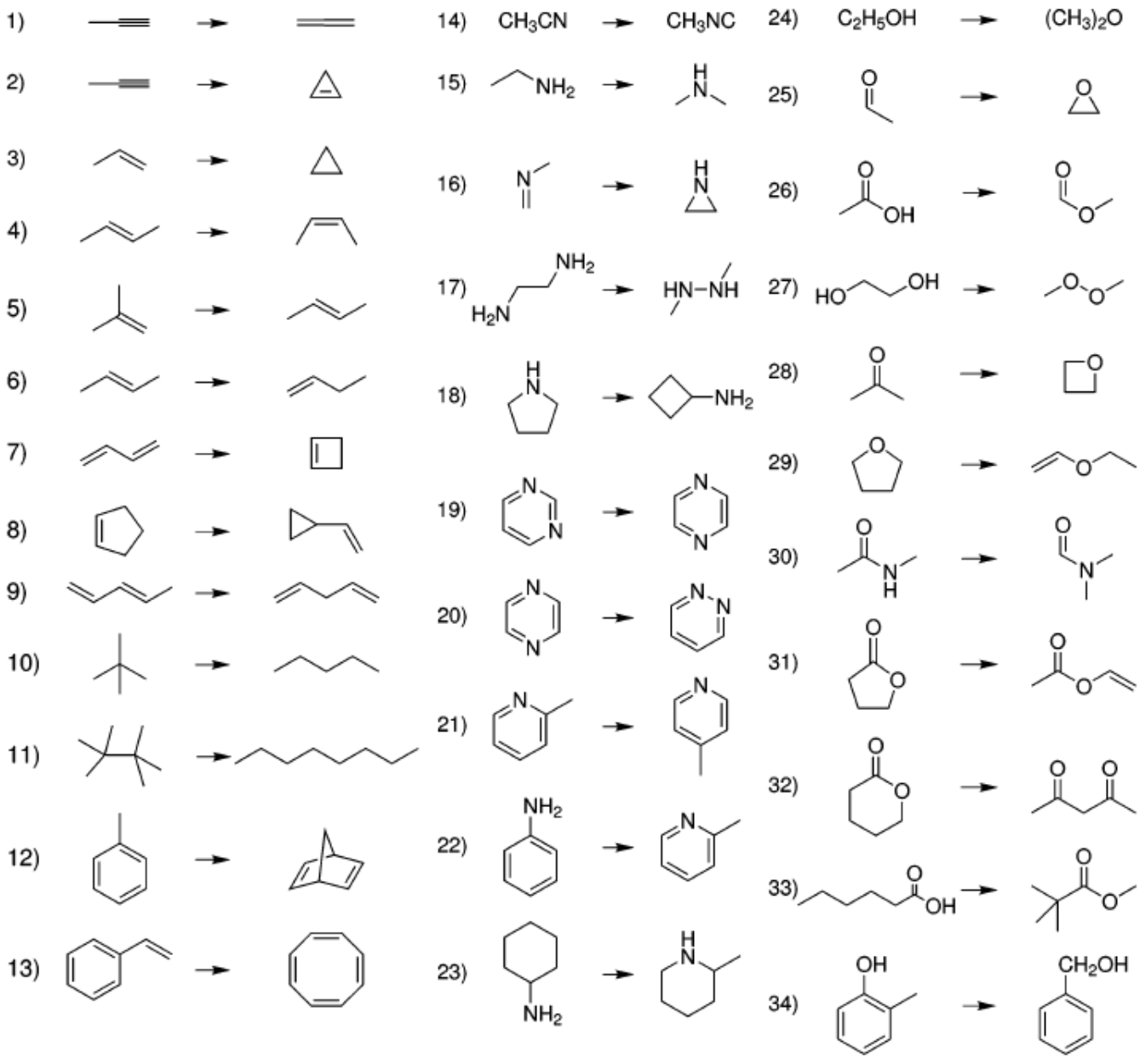
Dispersion dominated:



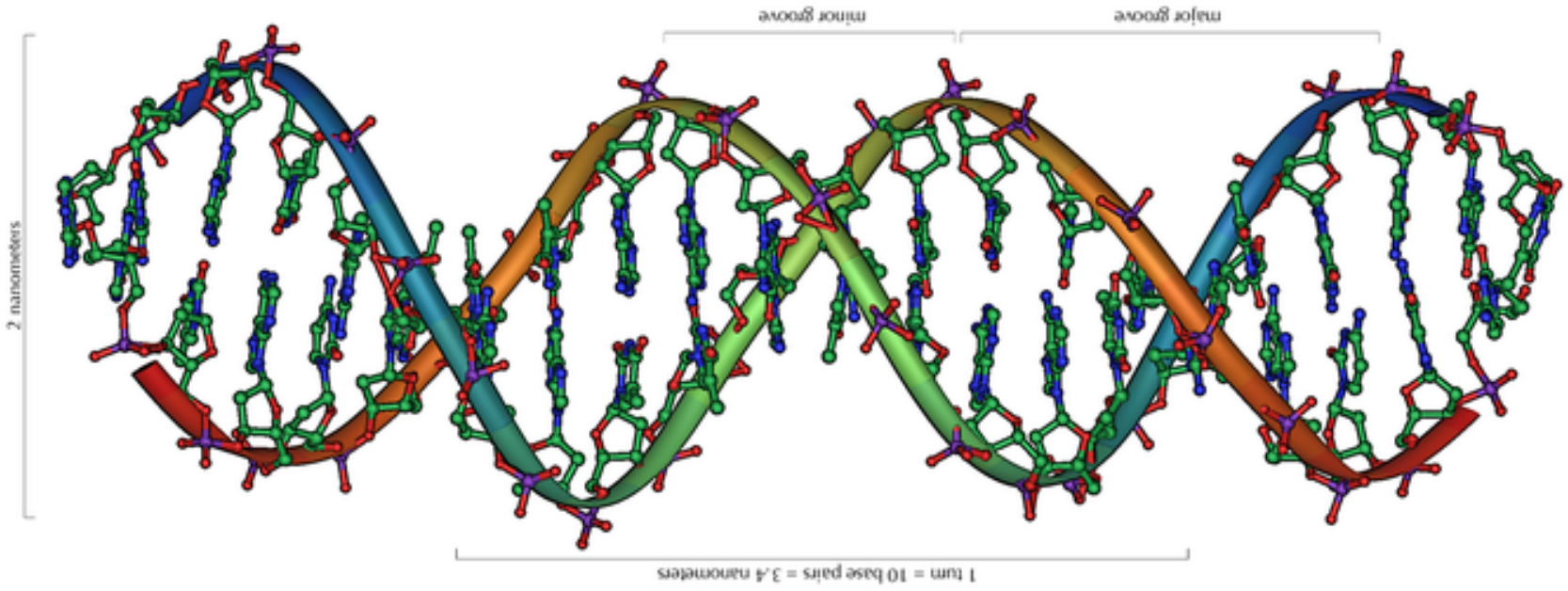
Mixed complexes:



benchmark reaction energies



accurate modeling of larger systems with FNDMC-QM/MM



... work in progress ...

Technical aspects: QMC@HOME's new sidekick

- QMC and other computational methods for chemistry at the Grimme group, University of Münster (D)

- QMC for solid state physics at the Theory of Condensed Matter group, University of Cambridge (UK)

Technical aspects: Current topics (2010)

Recent

- QuantumFIRE alpha test project for QMC in solid state physics and research into Quantum Foundations
- new main QMC app: CASINO (University of Cambridge, UK)
- additional QMC app: CHAMP (University of Twente, NL)
- new 'Pilot Wave Theory' app: LOUIS

Upcoming

- enable the QMC@HOME screensaver for CASINO
- enable CASINO for GPU computing

Technical aspects: Future plans (2011)

Extending our capabilities

- chemistry apps
  (Density functional theory and semiempirical QM methods)
- solid state physics apps
  (Density functional theory)
- choose open source projects were possible

'Volunteer Chemistry Initiative'

- supply ready-to-go packages for Volunteer Computing with standard chemistry codes including a screensaver framework
- sponsors welcome ...

Acknowledgments

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