A practical introduction to QM/MM using CP2K for biomolecular modelling

Reusing this material

The basics

- CP2K is an open-source quantum chemistry and solid state program.
  - Particularly well-liked for its density-functional theory (DFT implementations
  - Can be downloaded from:
    https://www.cp2k.org/download
- Everything we are covering today (and a lot of other info) can be found in the CP2K Reference Manual:
  https://manual.cp2k.org/#gsc.tab=0

The aims of this course

During this course, we aim to teach:

- How to model chemical reactions using CP2K
- Some CP2K functionalities that we find useful for biochemical QM/MM simulations
- The intricacies of running CP2K on a HPC facility

What we will not cover:

- Underlying computational chemistry theory and its implementation – this course is more practical-minded than theoretical
- How to choose the best QM/MM approach
- If you want more theory, we strongly recommend these following course:
  - Intro to QM/MM: https://www.youtube.com/watch?v=kZrGWcVcuFM

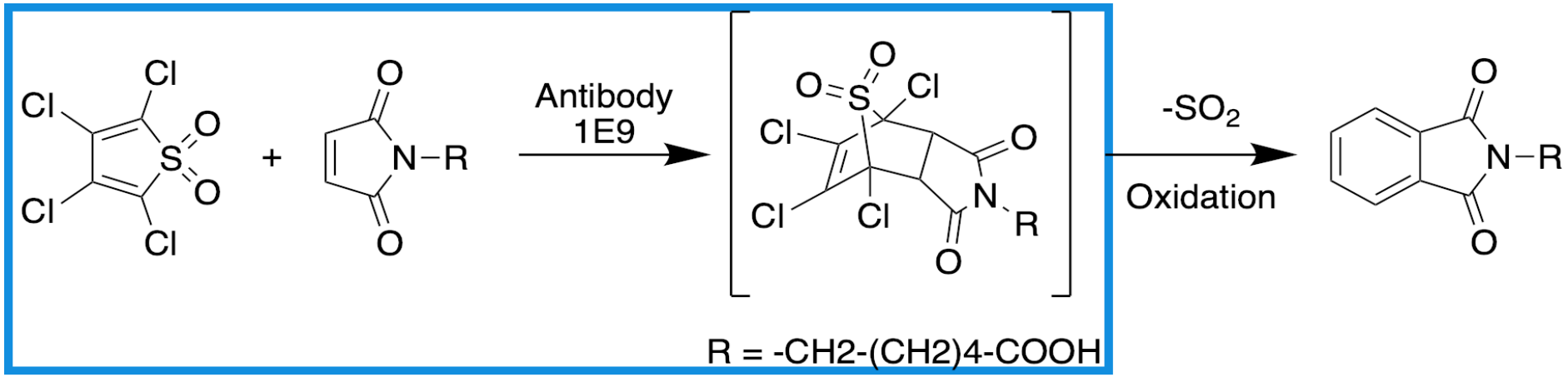
Overview of this session

- Introduction to CP2K
- The Diels-Alder reaction
- Running CP2K on ARCHER
  - Geometry optimisation simulations
    - Practical exercise
  - The DIMER method
- Coffee break
- The nudged elastic band method
  - Running a nudged elastic band simulation on CP2K
- Overview & questions

CP2K on ARCHER

- ARCHER uses modular packages
  - ARCHER has pre-installed versions of CP2K as a module
- Multi-processor jobs on ARCHER should:
  - Have the required modules loaded
  - Be submitted to backend nodes *via* submission script
  - Have a number of 24-processor nodes assigned
  - Be assigned a run time

Diels-Alder reaction

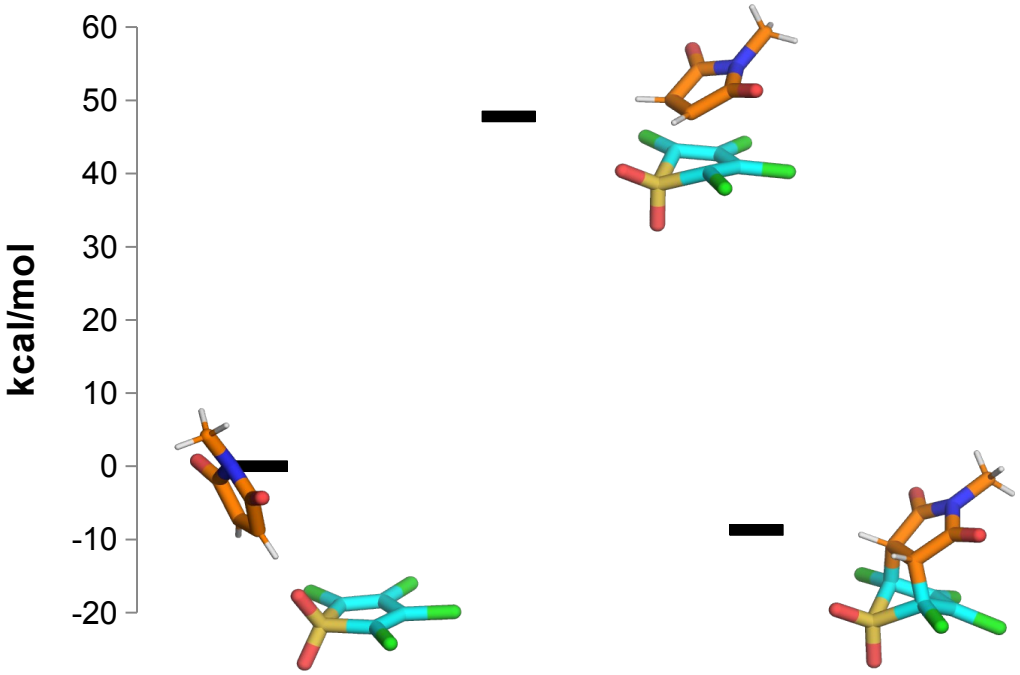


Science (1999) 286, 5448, 2345-2348

Geometry optimisation methods

Objectives:

- Optimise the reactant and product states
- Optimise the transition state using the DIMER method
- Check the optimised transition state with vibrational analysis



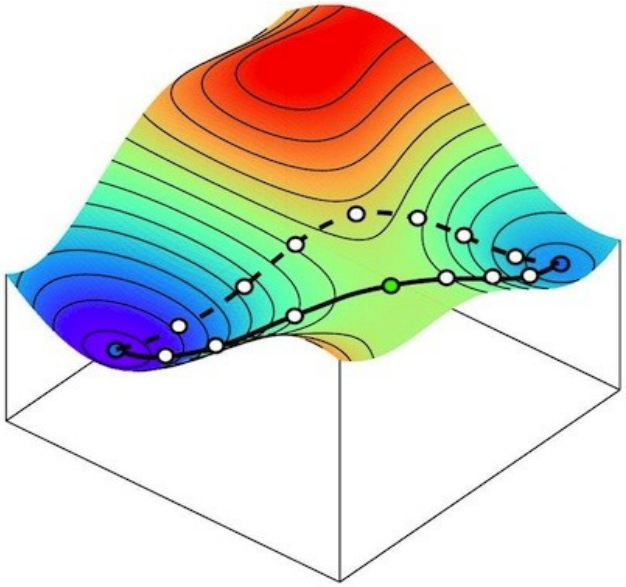
The nudged elastic band method

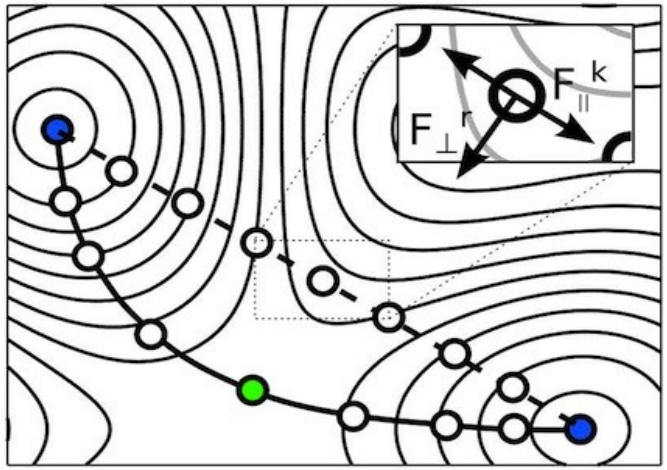
Nudged-Elastic Band (NEB) method

Chain-of-states method

Several geometries are used to describe the path between the reactant and product states. These images or geometries are linked by springs that constrain them to be separated from preceding and following configurations acting as an elastic chain.

- Simplest way to obtain images is linear interpolation of the initial and final geometries.
- Optimising this chain of configurations by only applying the component normal ($F_{\perp}^{r}$) to the reaction path ($F_{\parallel}^{k}$).





J. Chem. Phys. 113 (2000) 9901.

Overview for next session

- Questions from this session
- Filling the vacuum: the Diels-Alder reaction in solution
  - Preparing your QM/MM simulation with AmberTools
  - Setting up a QM region
  - Using metadynamics to speed up simulations
- Exercise session: the Diels-Alder reaction in a protein

Thanks for your time. Any questions?

Thanks also to:

- Clair Barrass for running the show behind the scenes
- Salome Llabres-Prat for doing a large amount of the preperation for this course
- Gerrit Groenhof who kindly gave us permission to use his Gaussian tutorial as a basis for this series.