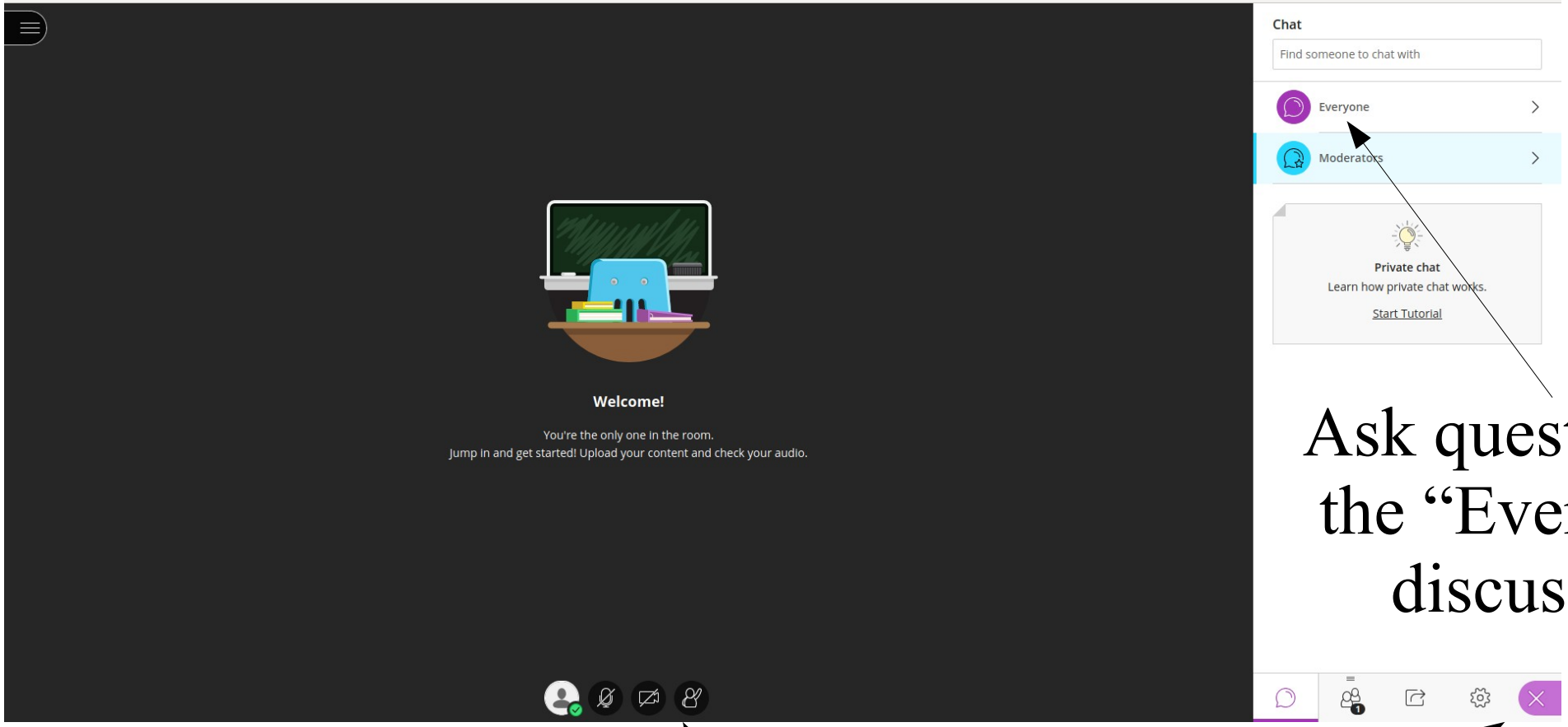
A practical introduction to QM/MM using CP2K for biomolecular modelling

Reusing this material

Using Collaborate

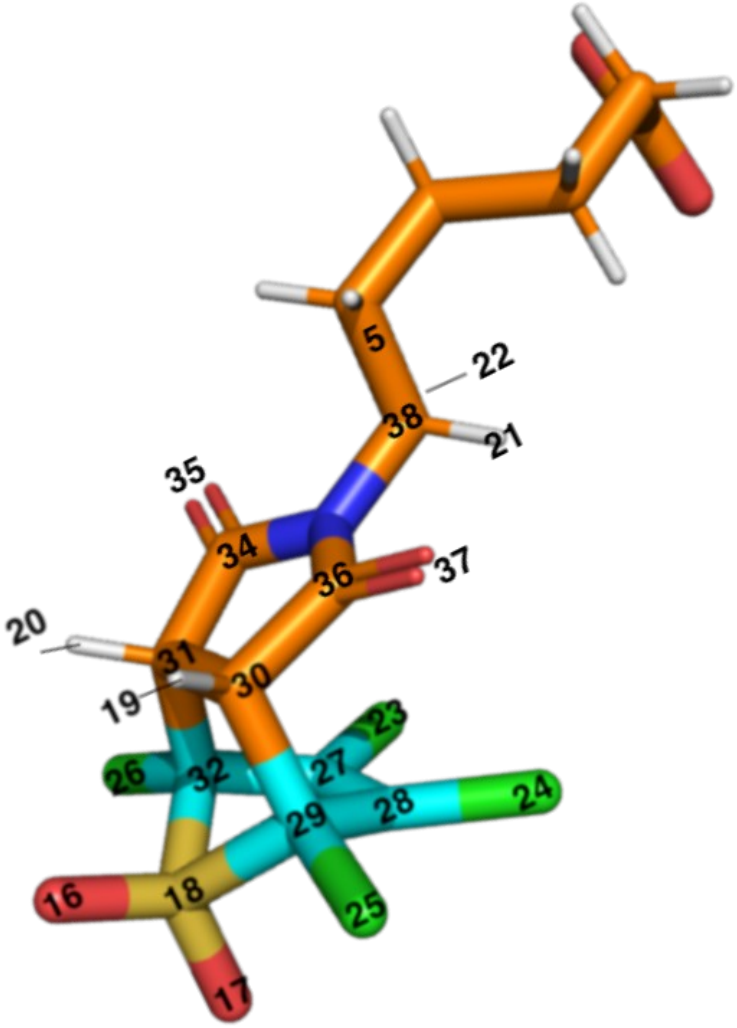


Ask questions in the "Everyone" discussion

Raise hands

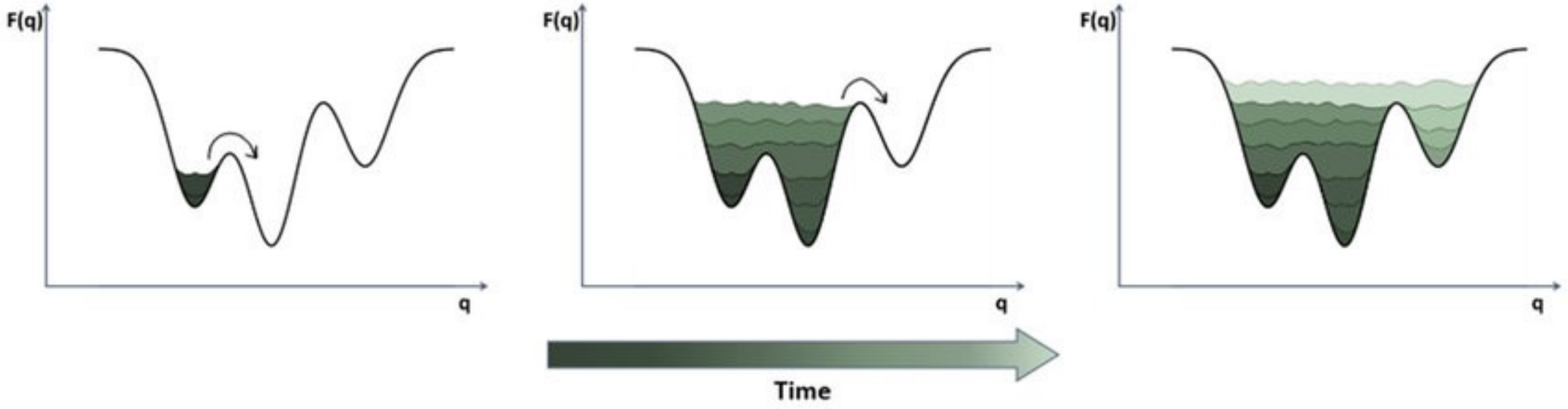
Bring out discussion tab

Overview of this session



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

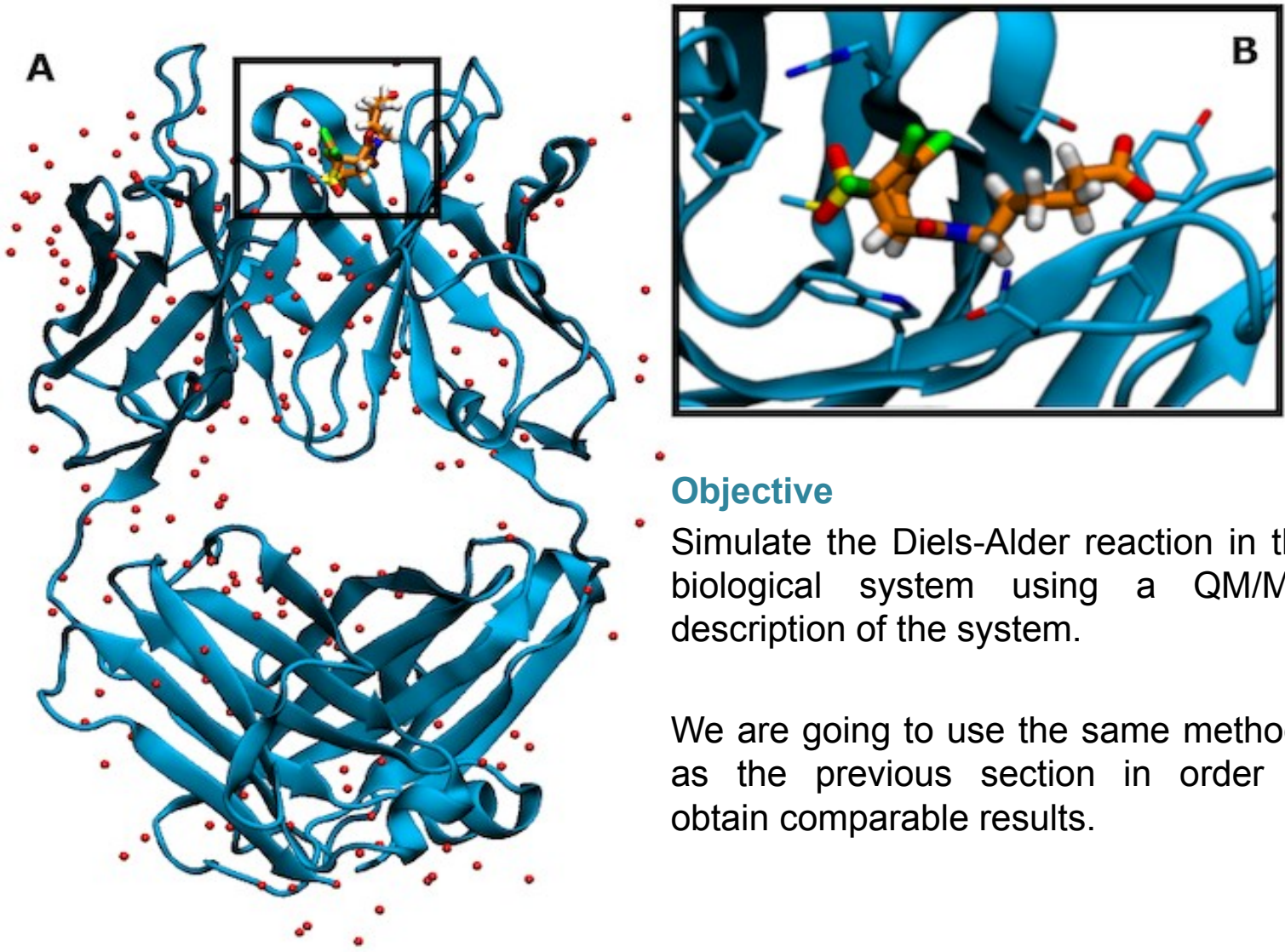
Metadynamics with Plumed



Finding collective variables

- The choice of collective variable (CV) is **crucial**
- CP2K provides a selection of Cvs here:
  - https://manual.cp2k.org/trunk/CP2K_INPUT/FORCE_EVAL/SUBSYS/COLVAR.html
- CP2K can also be linked with plumed to provide even more Cvs:
  - https://www.plumed.org/doc-v2.6/user-doc/html/colvarintro.html

Diels-Alder within a protein



Objective

Simulate the Diels-Alder reaction in the biological system using a QM/MM description of the system.

We are going to use the same methods as the previous section in order to obtain comparable results.

Certificate of Attendance exercise

- In Session 1 Exercise 3, when looking at the vibrational frequencies of the transition state, we used pre-set positions
- For this exercise, please use the positions obtained from the geometry optimisation of the transition state
  - You can either
    - copy-paste the positions in `DA.TS-pos-1.xyz`
    - Replace the FORCE_EVAL/SUBSYS/COORD section with a FORCE_EVAL/SUBSYS/TOPOLOGY section; add `COORD_FILE_FORMAT xyz` & `COORD_FILE_NAME name_of_file` to this section
- Send your input file and `DA.TS.freq-VIBRATIONS-1.mol` file to Training@epcc.ed.ac.uk

Further training opportunities

BioExcel training website
https://bioexcel.eu/services/training/

- In particular, note the Winter School on Biomolecular Simulations https://bioexcel.eu/events/winter-school/
- Also of note, a virtual workshop series on "Best Practices in QM/MM Simulations of Biomolecular Systems"
  - First session at 15:00 CET on Friday 30th October

ARCHER2 training website
https://www.archer2.ac.uk/training/

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.