QM/MM Simulation

Hybrid quantum mechanics/molecular mechanics (QM/MM) simulations have become a popular tool for investigating chemical reactions in condensed phases. In QM/MM methods, the region of the system in which the chemical process takes place is treated at an appropriate level of quantum chemistry theory, while the remainder is described by a molecular mechanics force field. Within this approach, chemical reactivity can be studied in large systems, such as enzymes. Using quality management to calculate the properties of a large chemical library is time-consuming and costly. High-precision QM/MM calculation is a multi-scale calculation method to study ligand binding. By using quantum chemistry representing ligands combined with molecular mechanics to characterize proteins and solvents, modeling time can be greatly reduced. Our bioinformaticians will provide you the most efficient quantum chemistry services.

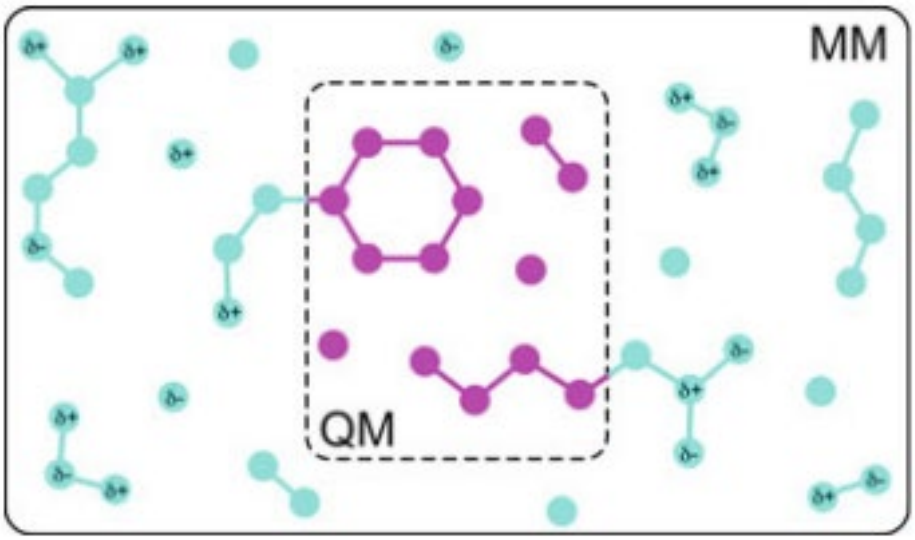


Figure 1. Illustration of the QM/MM concept. A small region, in which a chemical reaction occurs and therefore cannot be described with a force field, is treated at a sufficiently high level of QM theory. The remainder of the system is modelled at the MM level.

Overall solutions

- **Subtractive QM/MM Coupling**

  In the subtractive scheme, the QM/MM energy of the system is obtained in three steps. First, the energy of the total system, consisting of both QM and MM regions, is evaluated at the MM level. The QM energy of the isolated QM subsystem is added in the second step. Third, the MM energy of the QM subsystem is computed and subtracted. The last step corrects for including the

interactions within the QM subsystem twice:

$V_{QM/MM} = V_{MM}(MM+QM) + V_{QM}(AM) - V_{MM}(QM)$

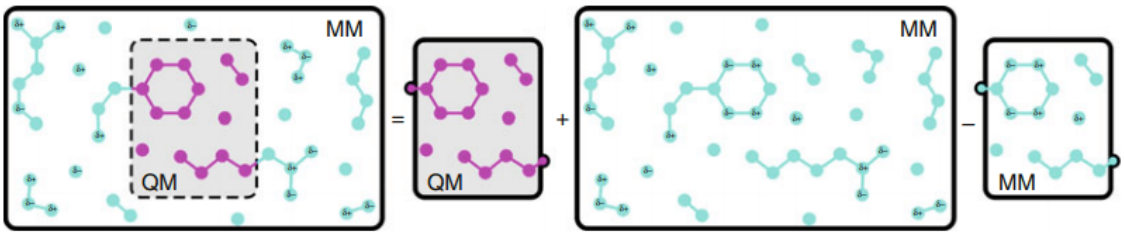


Figure 2. In the subtractive scheme, the QM/MM energy of the system is obtained in three steps.

QM and MM stand for the atoms in the QM and MM subsystems, respectively. The subscripts indicate the level of theory at which the potential energies (V) are computed. The main advantage of the subtractive QM/MM coupling scheme is that no communication is required between the quantum chemistry and molecular mechanics routines.

- **Additive QM/MM Coupling**

In additive schemes, the QM system is embedded within the larger MM system, and the potential energy for the whole system is a sum of MM energy terms, QM energy terms and QM/MM coupling terms:

$V_{QM/MM} = V_{QM}(QM) + V_{MM}(MM) - V_{QM-MM}(QM+MM)$

Here, only the interactions within the MM region are described at the force field level, $V_{MM}(MM)$. In contrast to the subtractive scheme, the interactions between the two subsystems are treated explicitly: $V_{QM-MM}(QM+MM)$

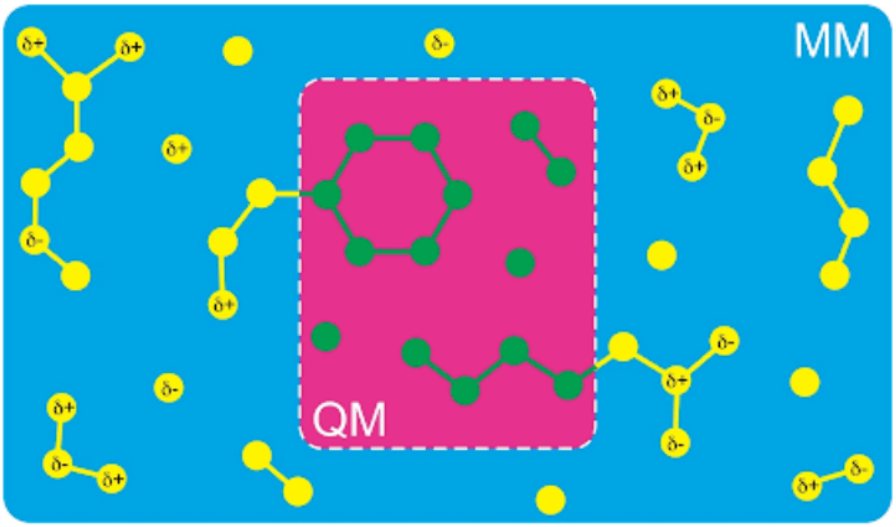
These interactions can be described at various degrees of sophistication.

Our services

Project name	QM/MM computing service
Samples requirement	Our QM/MM simulation service requires you to provide specific requirements.
Timeline	Decide according to your needs.
Deliverables	We provide you with raw data and analysis service.

Project name	QM/MM computing service
Price	Inquiry

Applications



- Molecular Dynamics Simulations

The QM/MM method provides both potential energies and forces. With these forces, it is possible to perform a molecular dynamics simulation.

- Geometry Optimization.
- Free Energy Computation.
- Free Energy Perturbation
- Computational Spectroscopy. (UV/vis Absorption Spectr and IR Absorption Spectra)

CD ComputaBio can offer you but not limited to:

- Density functional theory calculation
- Reverse virtual screening
- 3D-QSAR service
-

CD ComputaBio' QM/MM simulation service can reduce the cost of later experiments. QM/MM simulation service is a personalized and customized

innovative scientific research service. Before determining the corresponding analysis plan and price, each project needs to be evaluated.