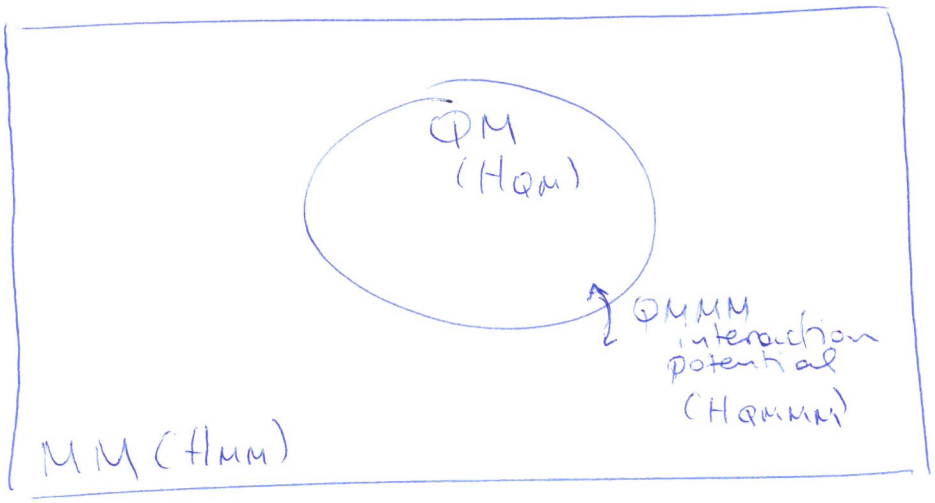
4.2 Quantum Mechanics - Molecular Mechanics (QM/MM)

Combine very accurate QM with classical MM.



Hamiltonian of the QM part: $\hat{H}_{QM} = \hat{T}_e + \hat{T}_k + \hat{V}_{ek} + \hat{V}_{kk} + \hat{V}_{ee}$

(kinetic terms and interaction for electrons-e and nuclei-k)

$$\hat{H}_{QMMM} = H_{QM} - \sum_{km} \frac{Q_k e}{|\vec{R}_k - \vec{r}_m|} + \sum_{kL} \frac{Q_k Q_L}{|\vec{R}_k - \vec{R}_L|}$$

interactions of electrons in QM region with charges in MM region

interaction among charges of MM atoms

$$\hat{H}_{MM} = \hat{V}_{bonded} + \hat{V}_{non-bonded}$$

The interface between QM and MM should be treated (and set) with care.

When bonds across the interface are formed:

- the valence of the QM part should be satisfied
- The MM bonding terms should have a partner term in the QM part to maintain the geometry

Methods for bond treatment across the interface
- Link atoms
- local self-consistent
- generalized hybrid orbital

Drawbacks of QMMM
- parameterization still required for interface treatment
- choice of QM size not easy
- QM region polarizes in response to MM partial charges, but not the inverse.