

NATURE



Born-Oppenheimer approximation
Limited treatment of QM (DFT or semiempirical)
Implicit treatment of some electrons

QM/MM



Implicit representation of all electrons

**POLARIZABLE
MM**



Neglect of polarization
Representation of multipolar moments
by fixed charges

MM



Rigid receptor
Rigid or semi-rigid ligand
Single-configuration scoring
Simple solvation model

DOCKING