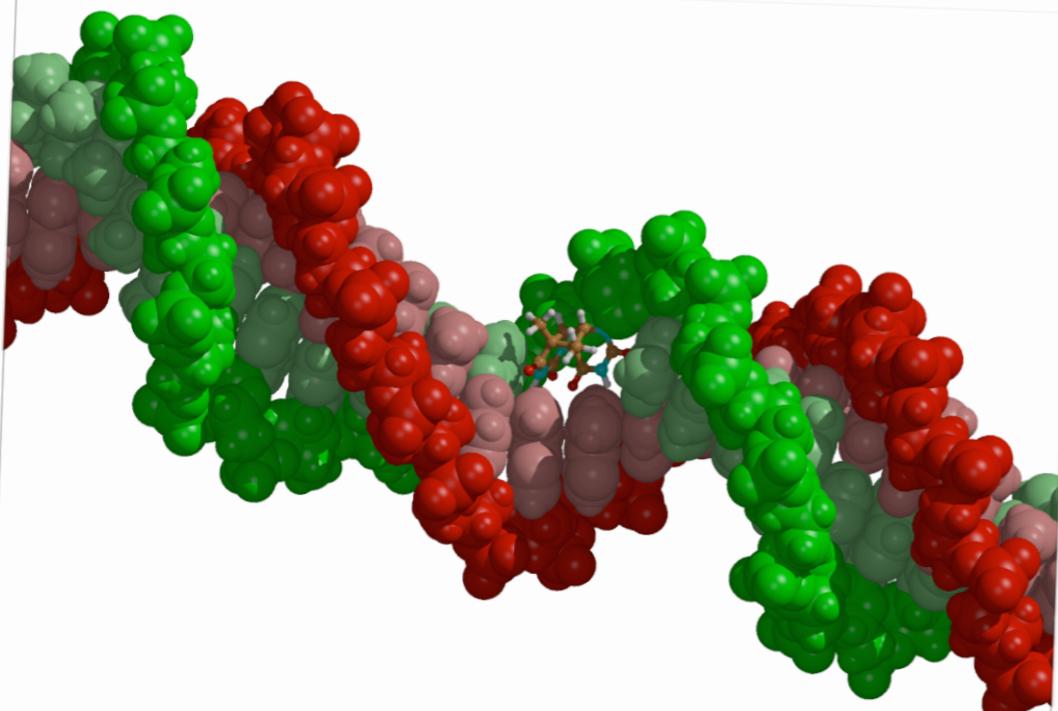
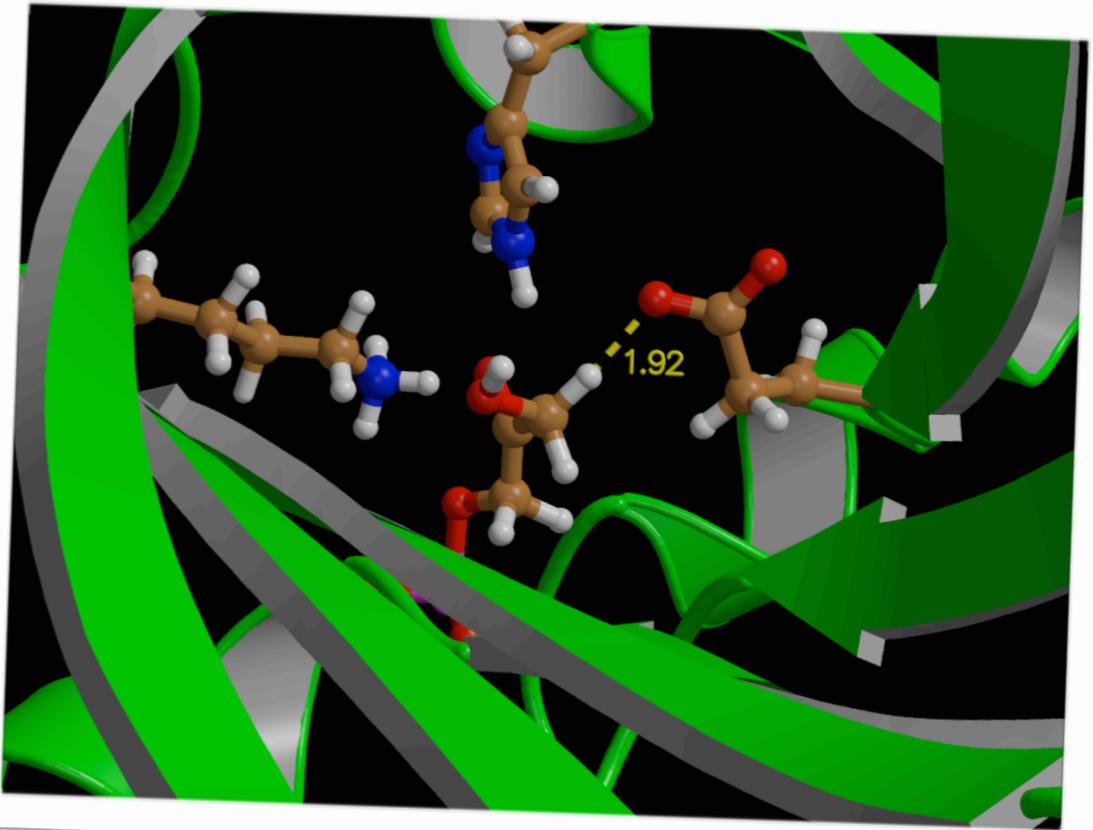


photochemistry/photobiology



radiation damage



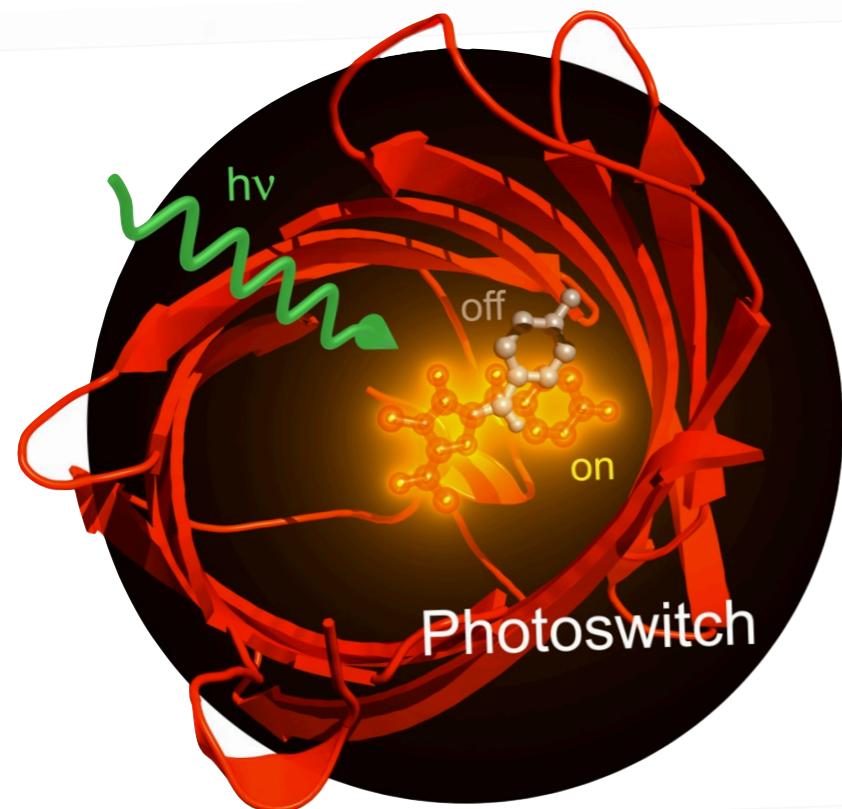
enzyme catalysis

```
real calculate_QMMM(rvec x[],rvec f[], t_forcerec *fr,t_mdatoms *md)
{
    real
        QMener=0.0;

    QMener = call_QMroutine cr,fr,qm,mm,forces,fshift);

    for(i=0;i<qm->nrQMatoms;i++)
    {
        for(j=0;j<DIM;j++)
        {
            f[qm->indexQM[i]][j]           -= forces[i][j];
            fr->fshift[qm->shiftQM[i]][j] += fshift[i][j];
        }
    }
    for(i=0;i<mm->nrMMatoms;i++)
    {
        for(j=0;j<DIM;j++)
        {
            f[mm->indexMM[i]][j]           -= forces[qm->nrQMatoms+i][j];
            fr->fshift[mm->shiftMM[i]][j] += fshift[qm->nrQMatoms+i][j];
        }
    }
    return(QMener)
}
```

method development



biology and nanotechnology

protein environment

experimental groups: Klaas Hellingwerf, Marloes Groot

tomorrow

bio- & nanotechnology

design

examples

bacteriorhodopsin

photoactive yellow protein

green fluorescent protein

Photochemistry

at the interface between biology and nanotechnology

today

photobiological reactions

understand the effect of protein environment

experimental groups: Klaas Hellingwerf, Marloes Groot

tomorrow

bio- & nanotechnology

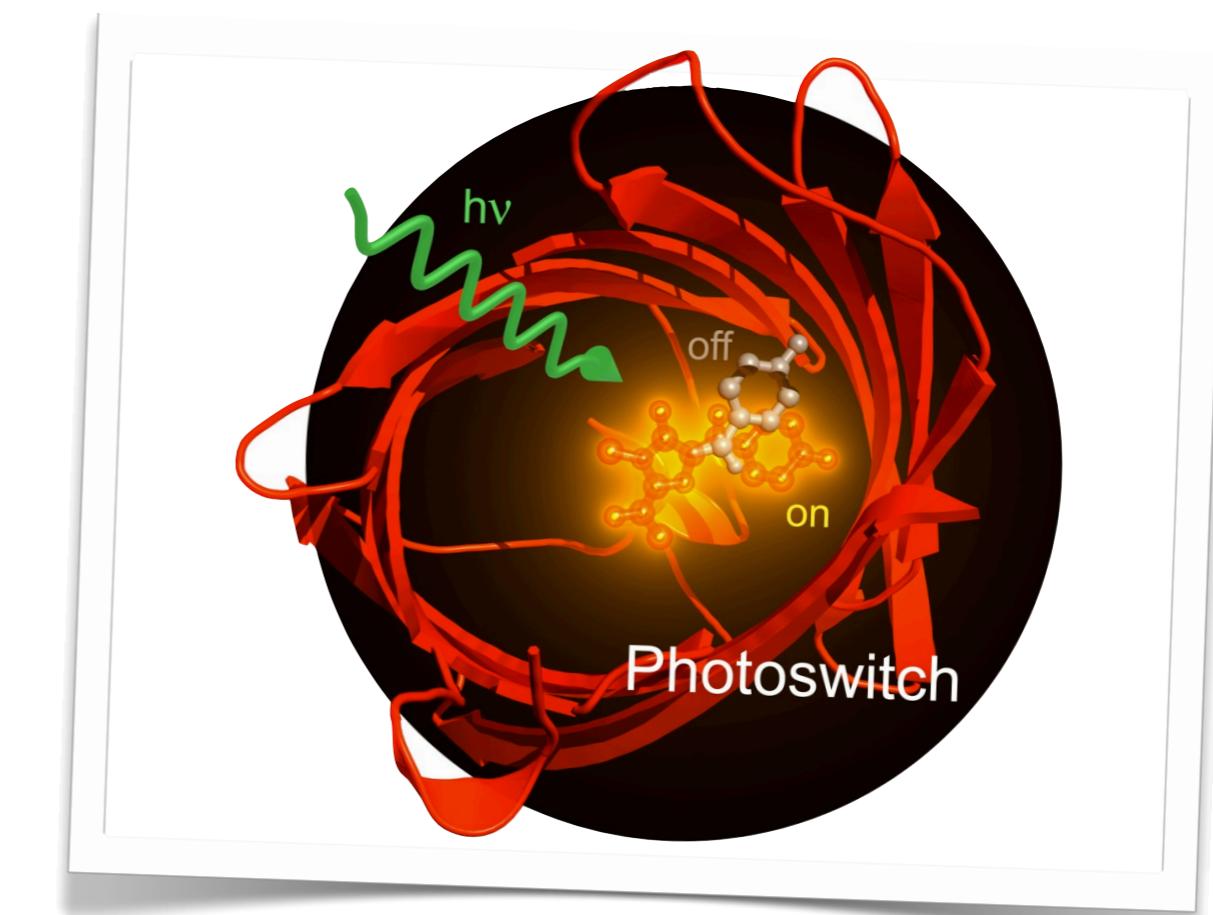
design

examples

bacteriorhodopsin

photoactive yellow protein

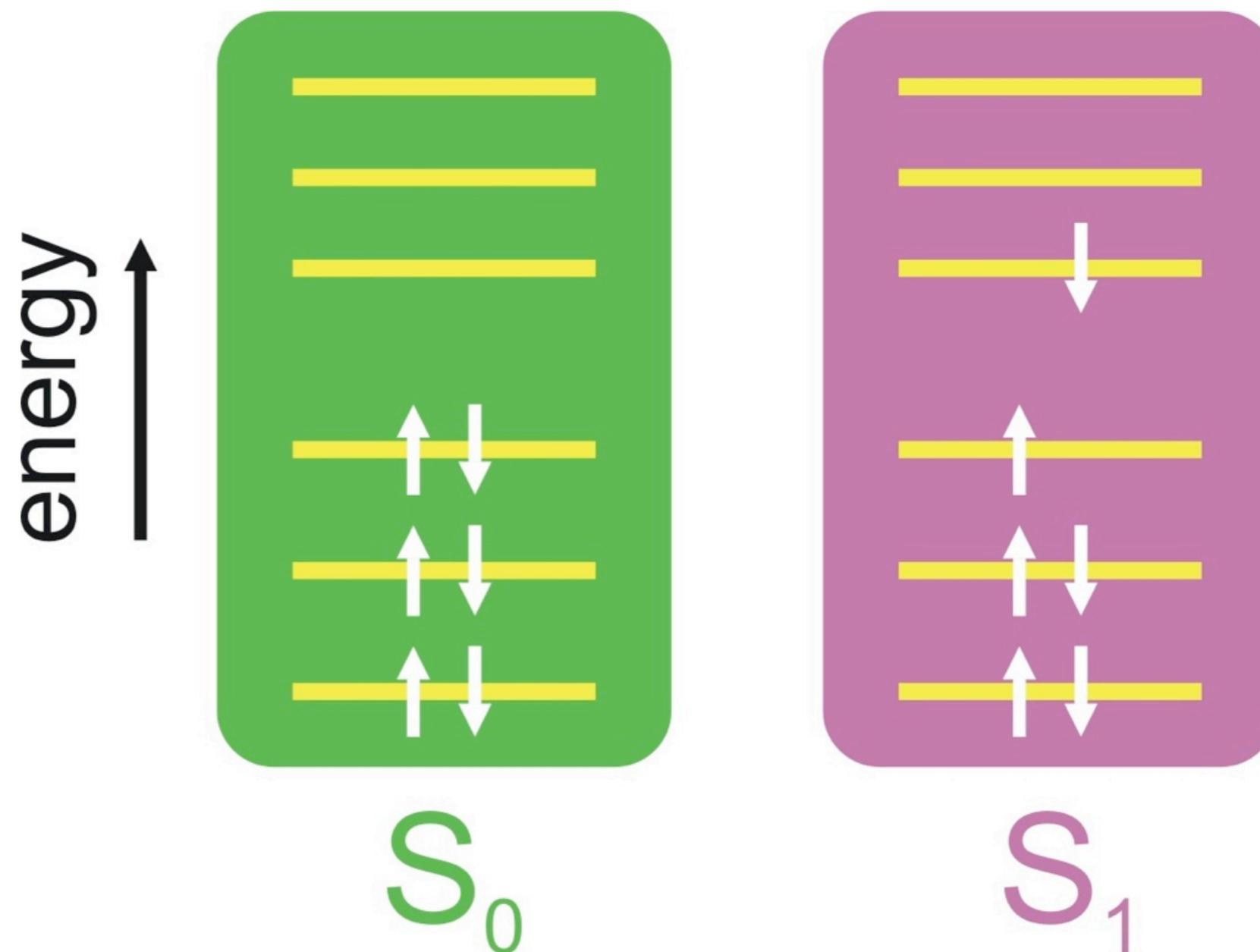
green fluorescent protein



Principles of photochemistry

electronic excitation

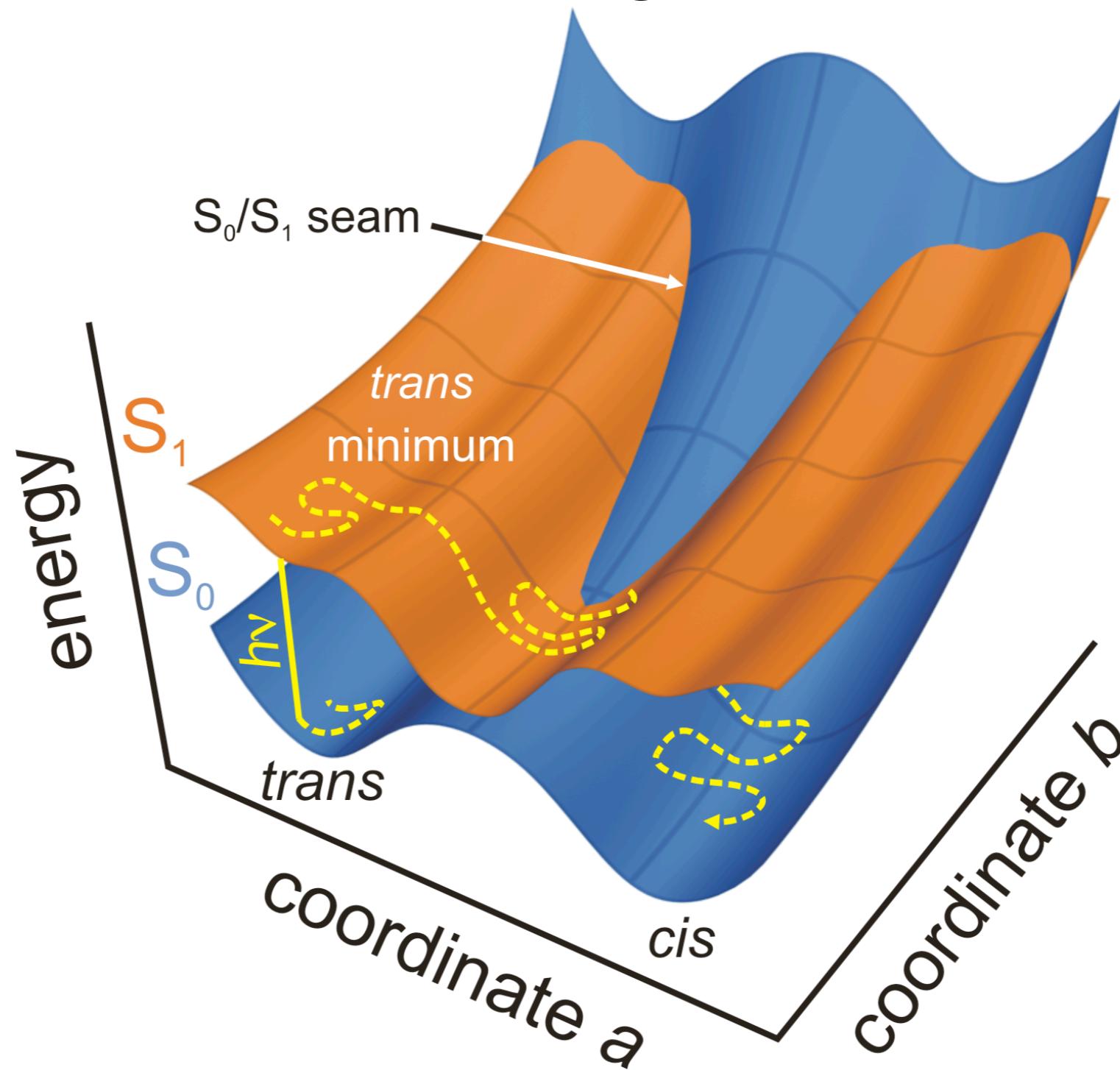
multi-reference methods: CASSCF/CASPT2/...



Principles of photochemistry

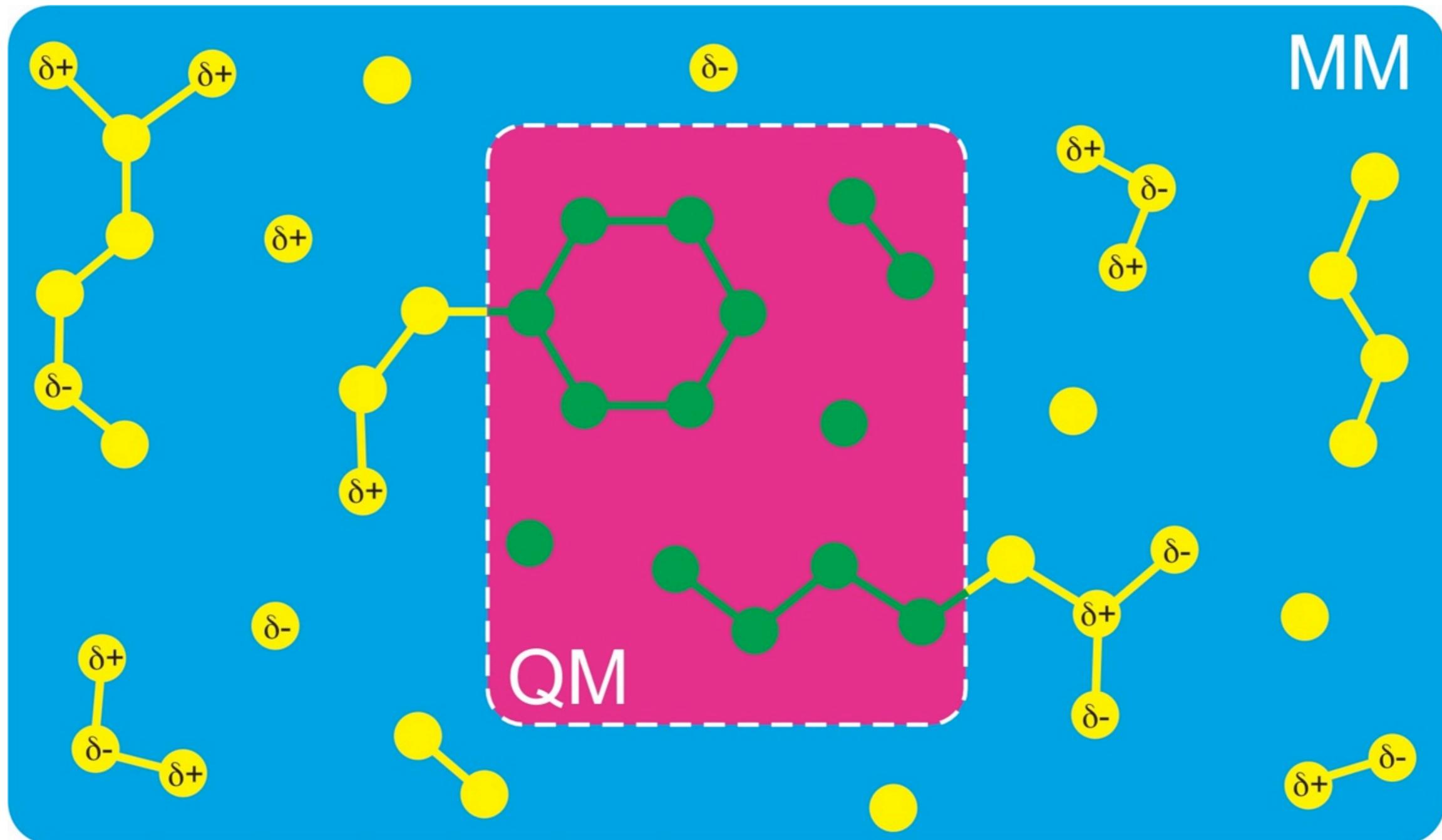
excited state potential energy surface (S_1)

non-adiabatic transitions to ground state surface (S_0)



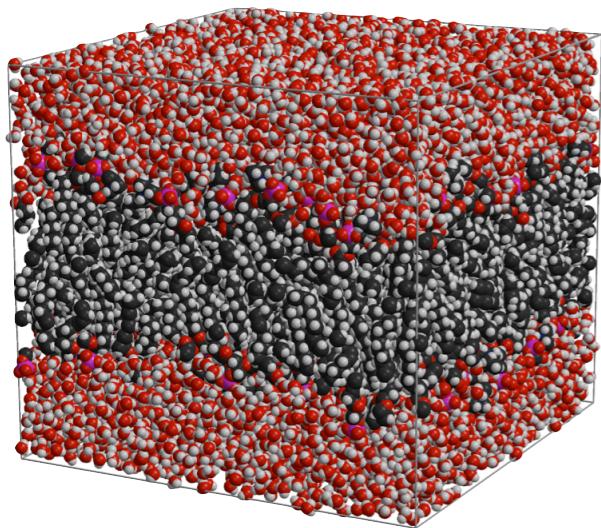
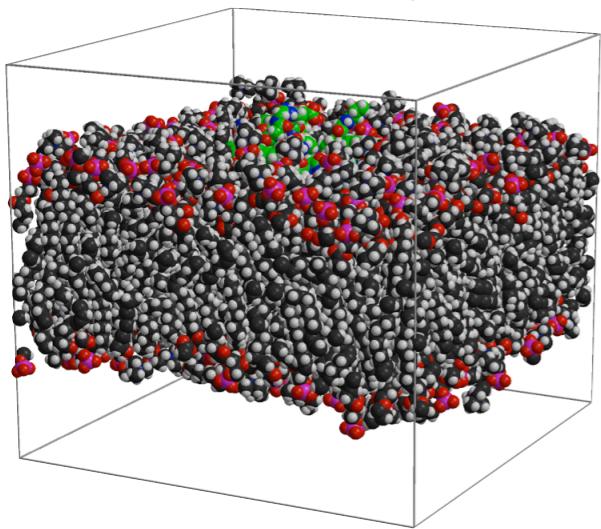
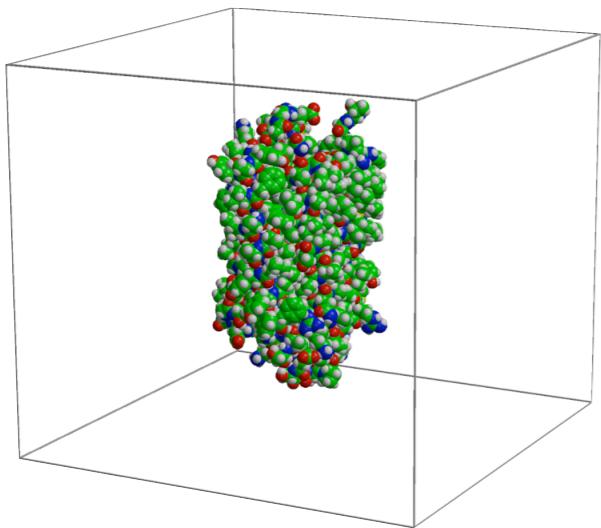
Modeling condensed-phase photochemistry

hybrid quantum mechanics/molecular mechanics



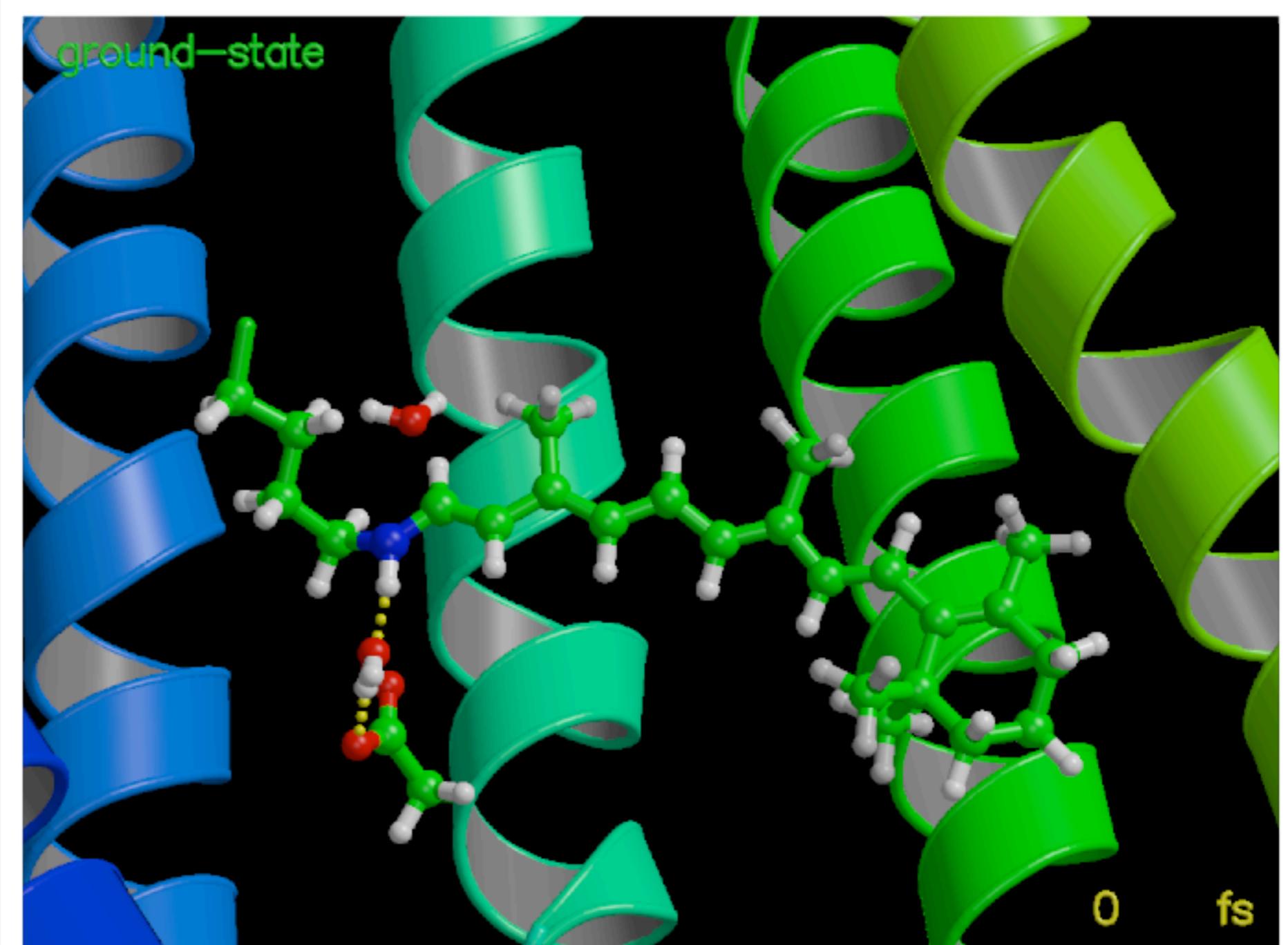
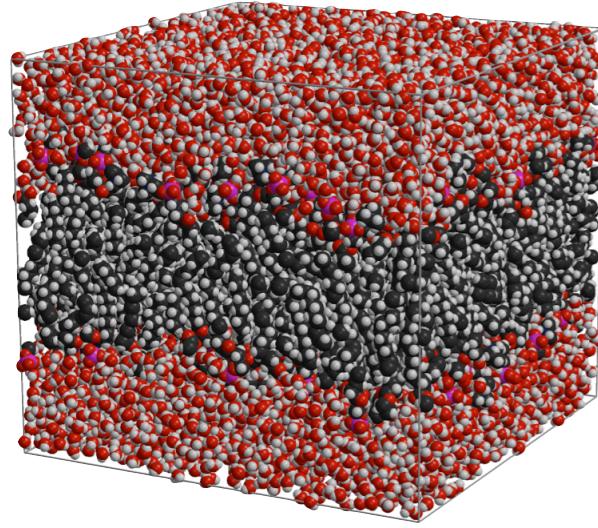
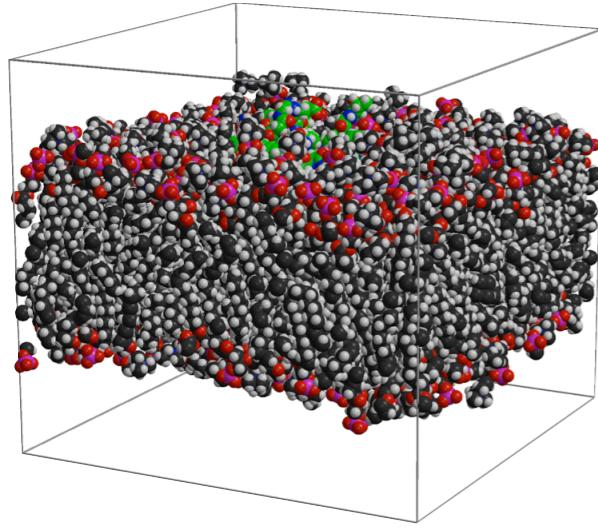
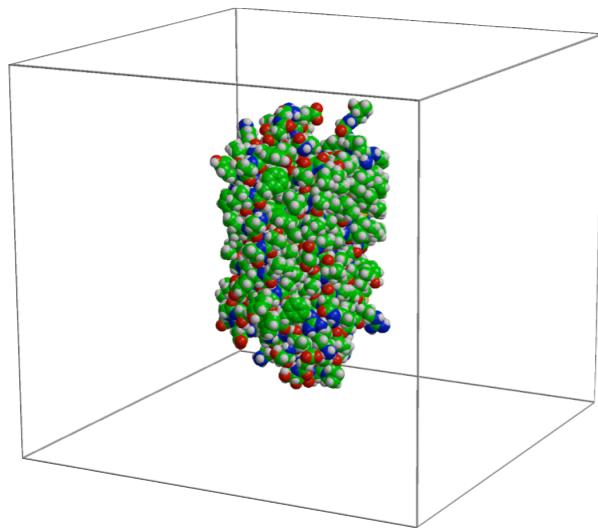
Observe while it happens: bacteriorhodopsin

catching the photo-isomerization of retinal in the act



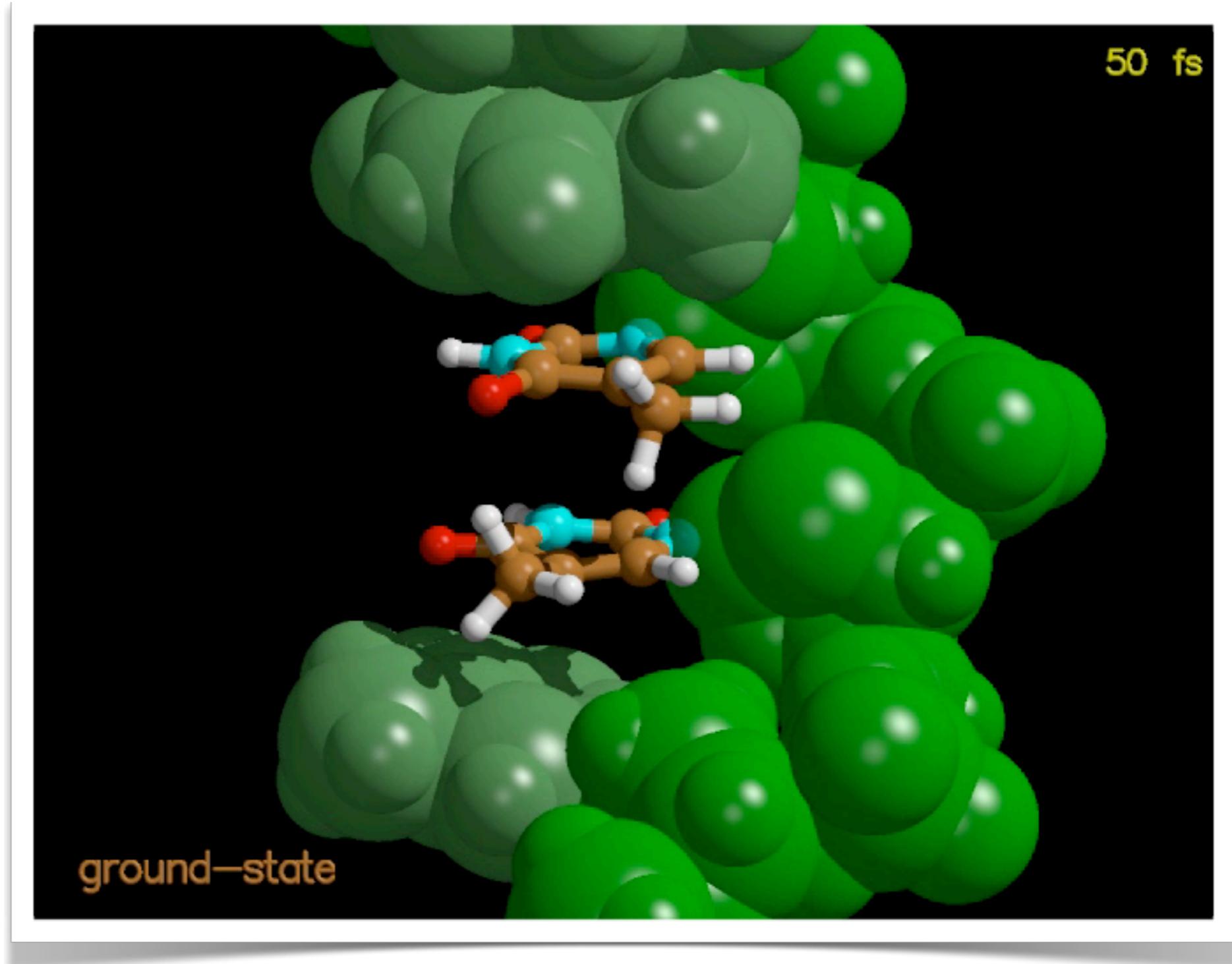
Observe while it happens: bacteriorhodopsin

catching the photo-isomerization of retinal in the act



Radiation damage: UV absorption in DNA

excited-state simulation of TT base stack



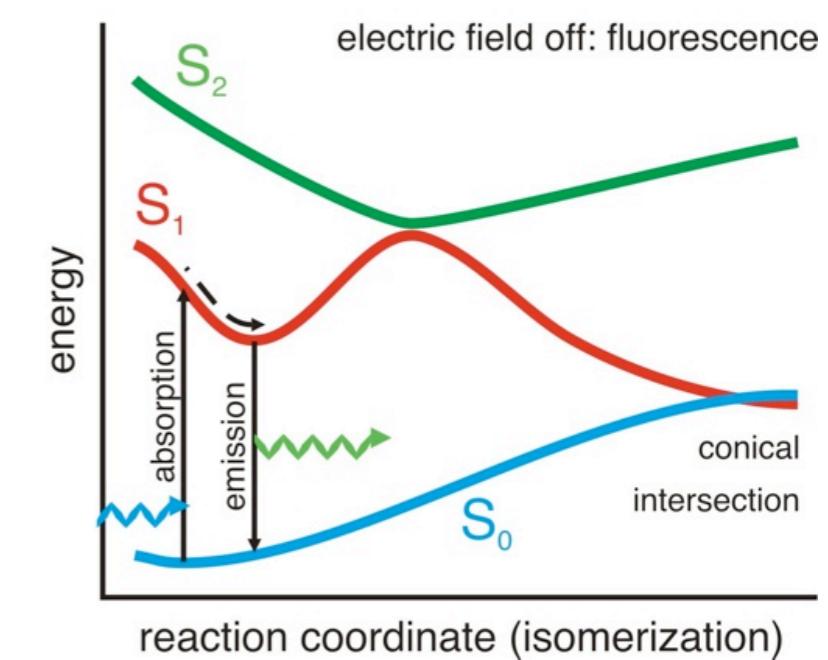
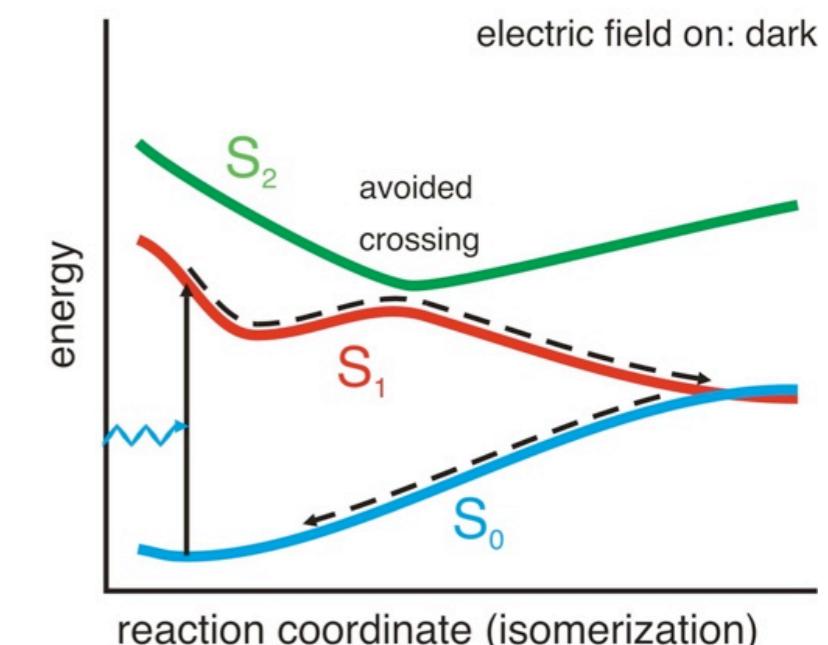
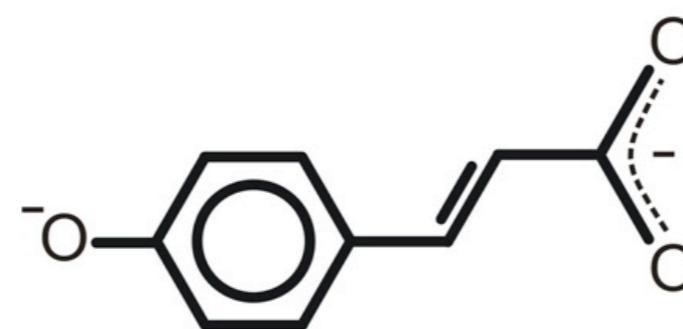
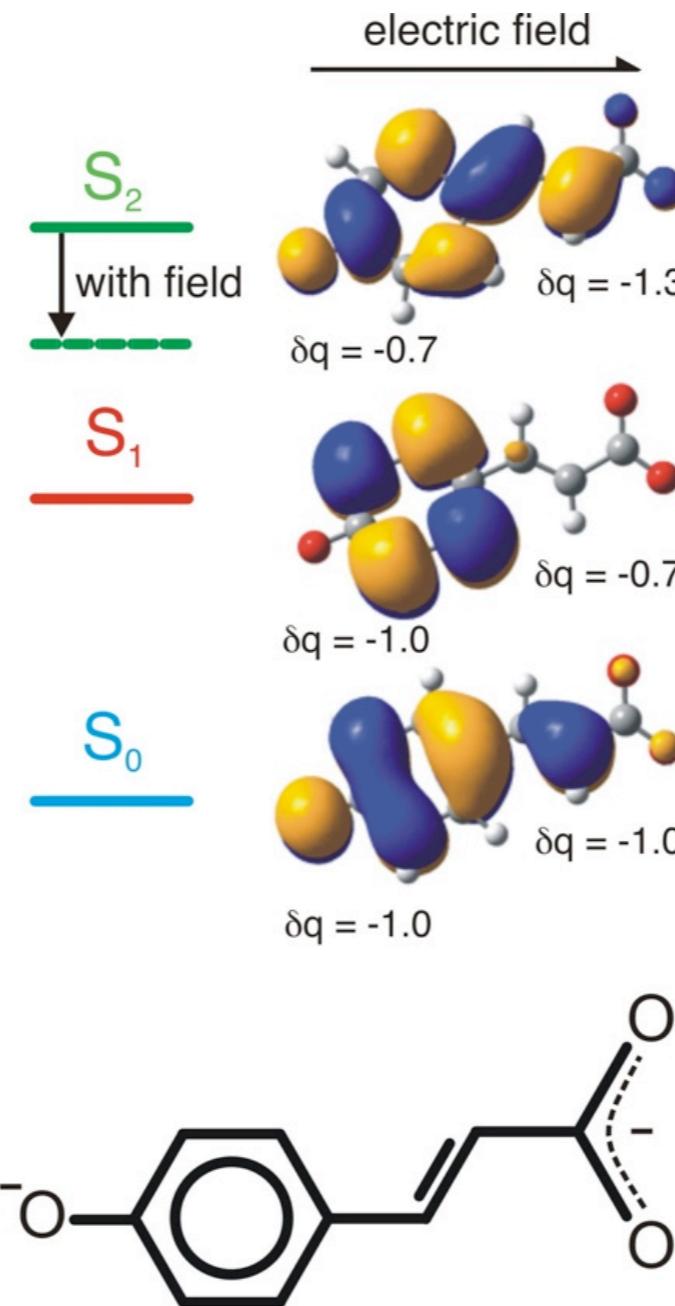
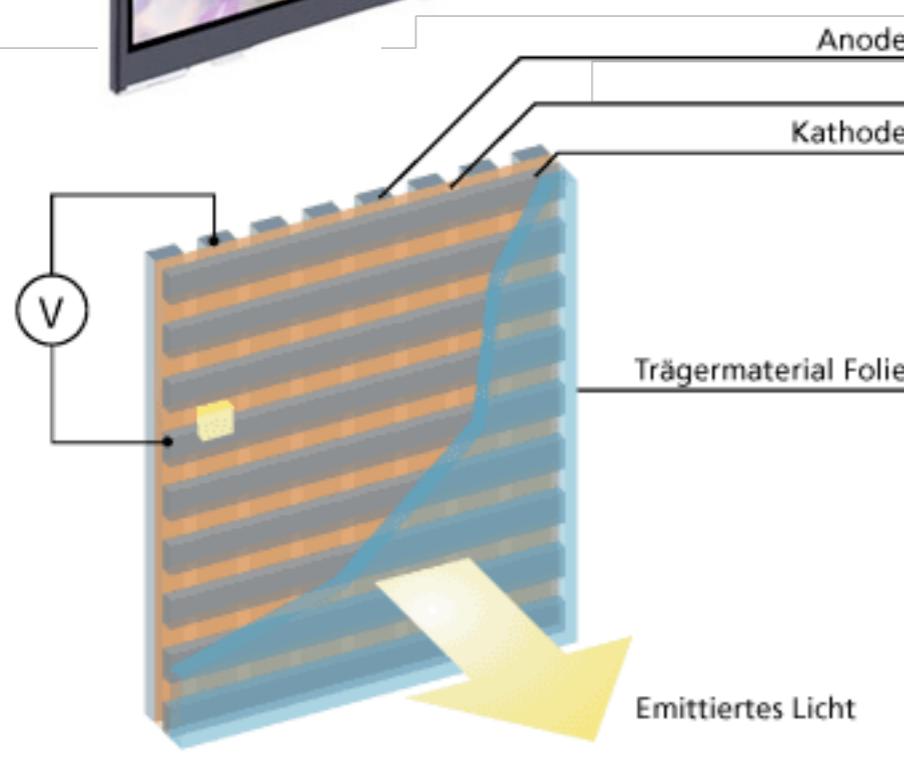
Possible bachelor projects

1. control of photochemistry by electric fields
2. biomimetic devices
3. effect of EPR probes on RNA structure & dynamics
4. influence of pH on peptide folding
5. proton transfer in classical Molecular Dynamics

Possible bachelor projects



Timo Grän

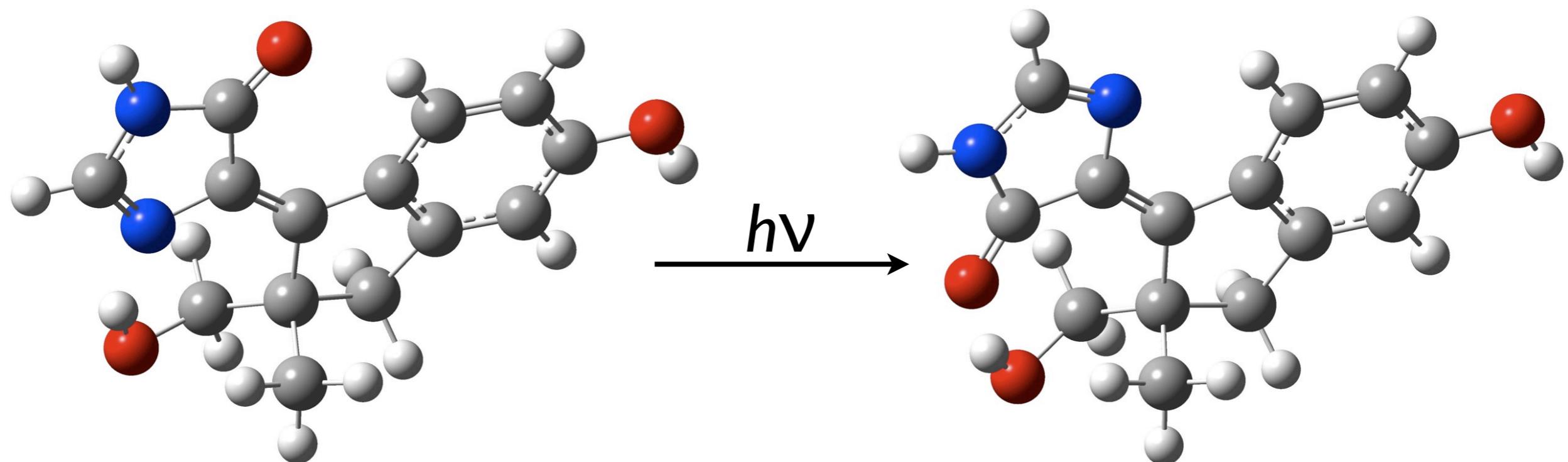


Possible bachelor projects

2. biomimetic devices

switchable fluorescent proteins (GFP, Dronpa, asFP)

pK_a shift upon photo-isomerization

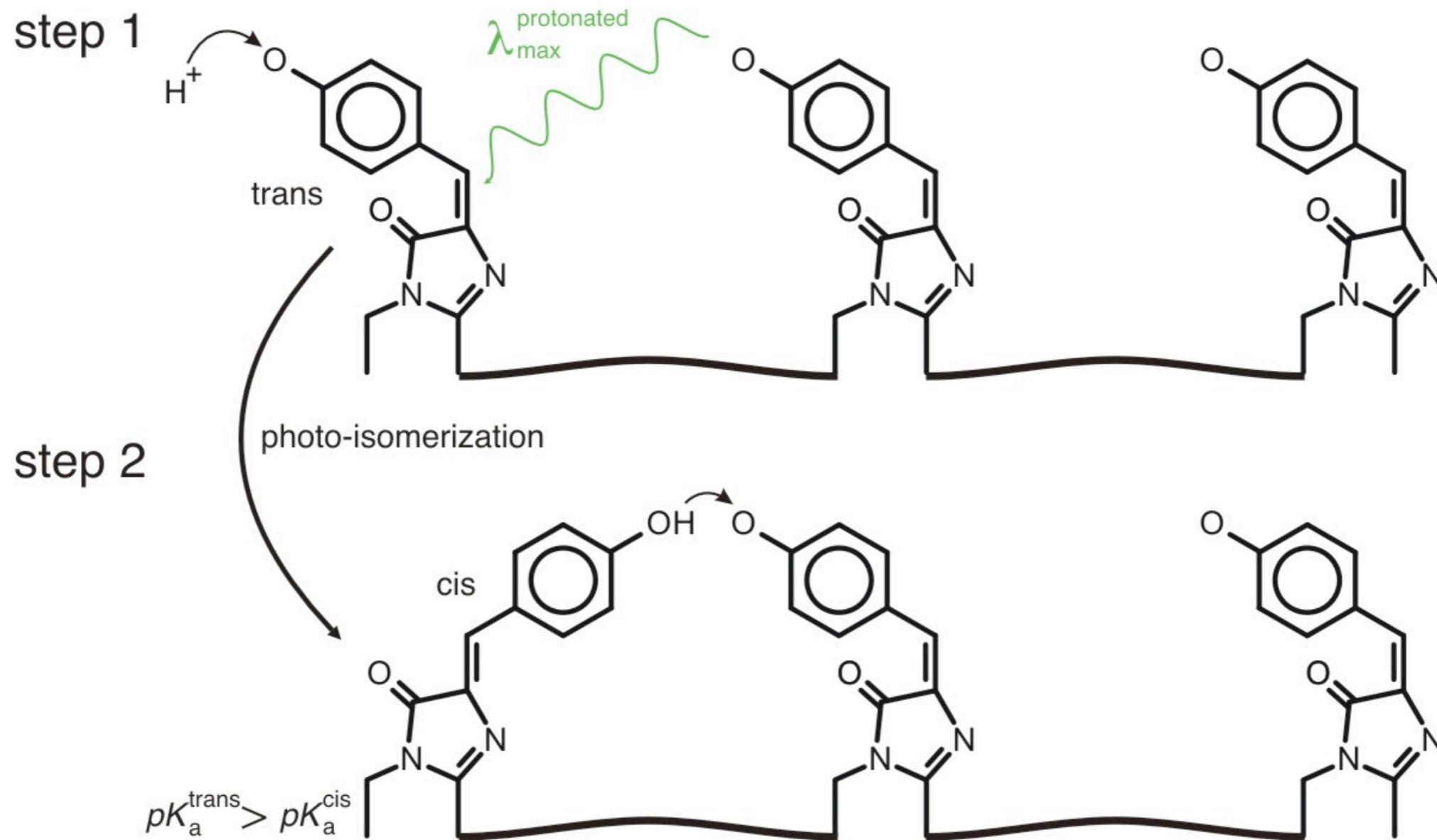


$\Delta pK_a \approx 1$ unit (in vacuum)

Possible bachelor projects

2. biomimetic devices

long-term goal: active proton transport

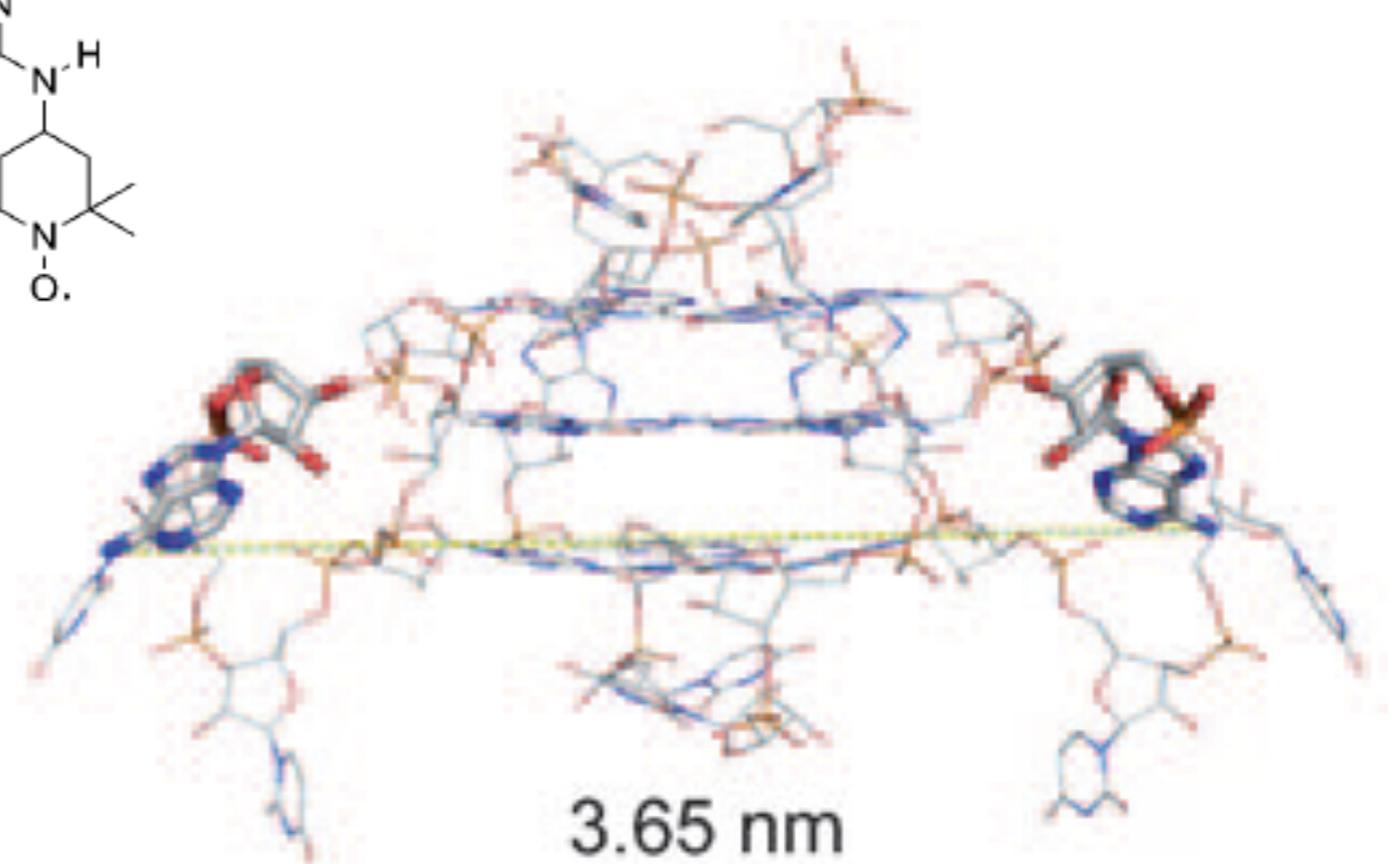
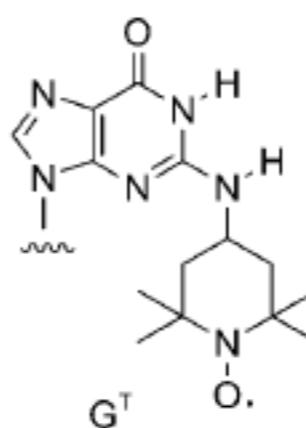
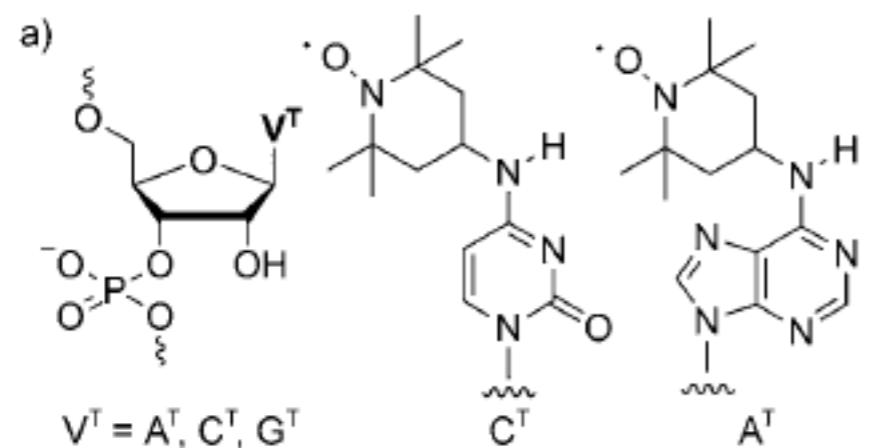


Possible bachelor projects

3. effect of EPR probes on RNA structure & dynamics

pulsed EPR measures distances

TEMPO probe



Claudia Höbartner
Marina Bennati

Possible bachelor projects

4. influence of pH on peptide folding

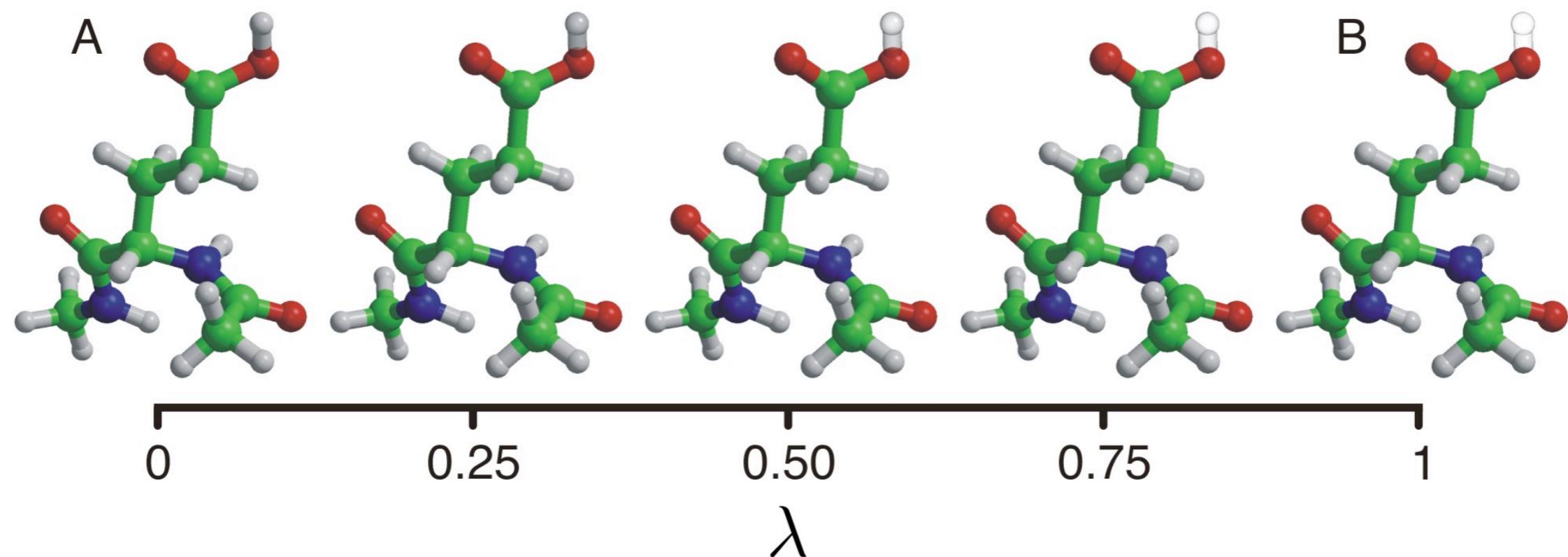
$$\text{pH} = -\log[\text{H}^+]$$



Serena
Donnini

molecular dynamics at constant pH

λ -dynamics: protonation as extra degree of freedom



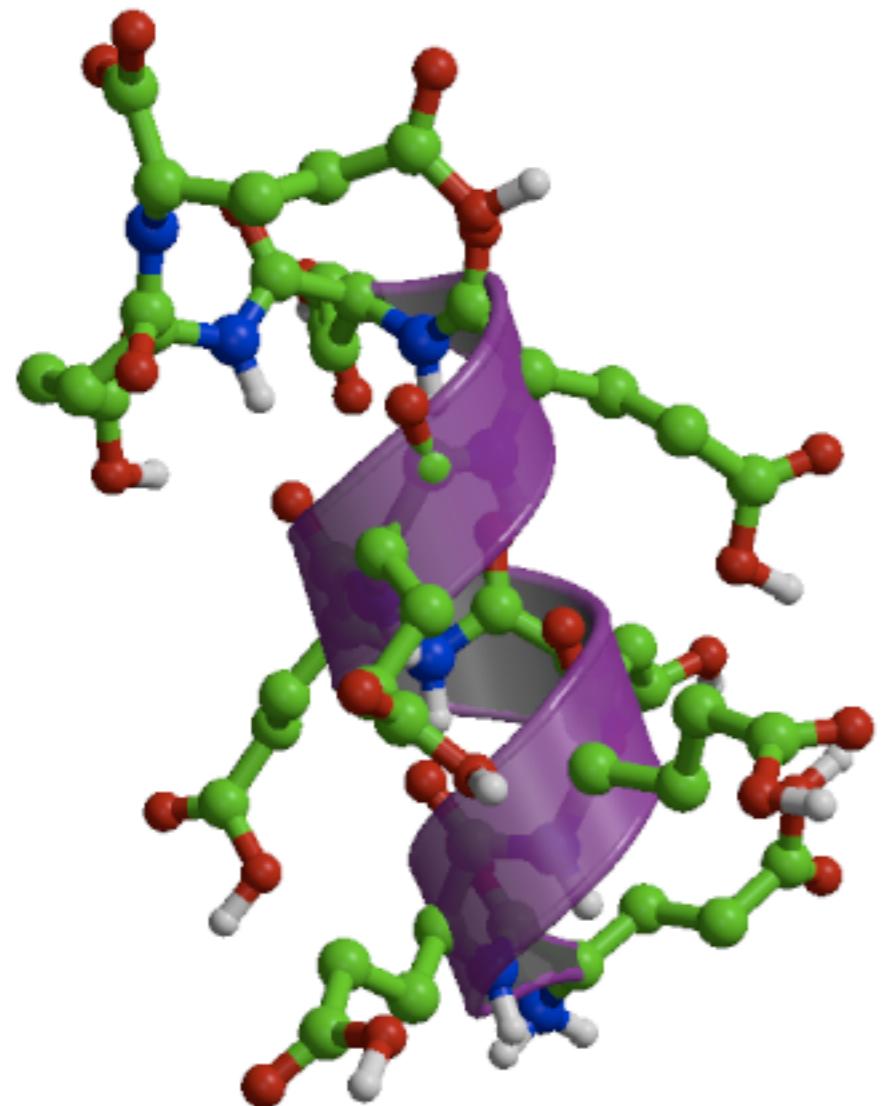
Possible bachelor projects

4. influence of pH on peptide folding

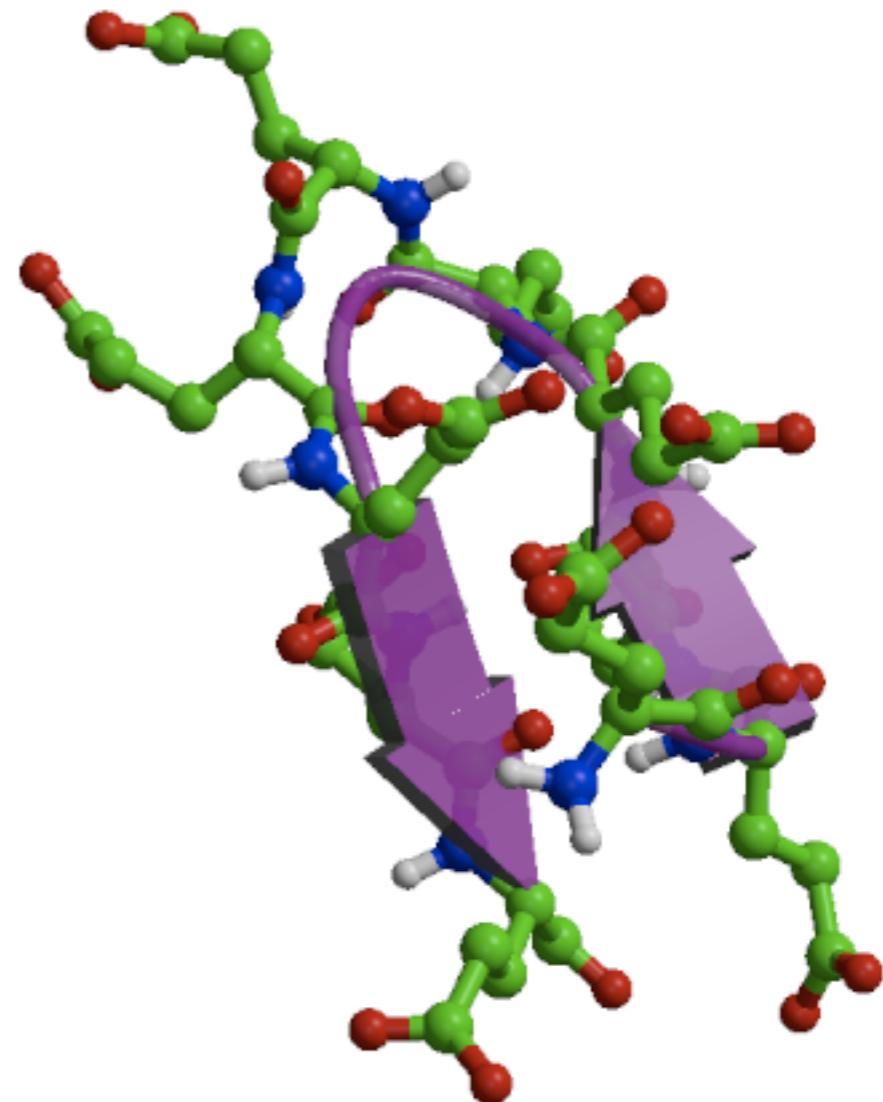
conformation as function of pH: Glu₁₀



Serena
Donnini



low pH: acidic



high pH: basic

Possible bachelor projects

5. proton transfer in classical MD

λ -dynamics: proton transfer reaction coordinate

testing & further implementation



Maarten
Wolf

