Photochemistry of Proton Transfer with Tensor Networks

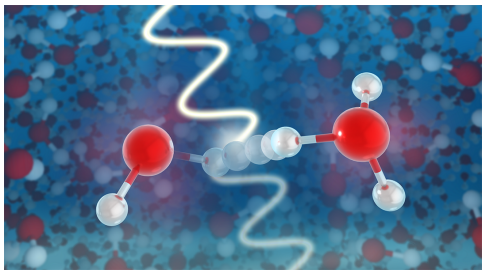


Figure: Proton transfer in biological medium (Image by Argonne National Laboratory)

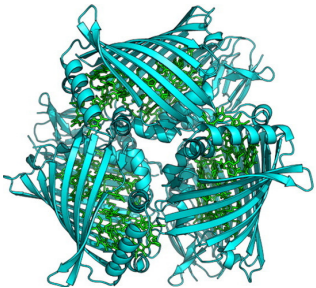
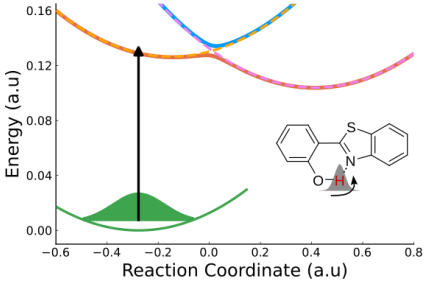
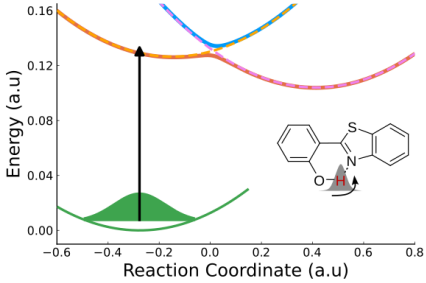


Figure: Crystal structure of an FMO pigment system, where proton transfer takes place

Brieuc LE DE (INSP), Alex CHIN (INSP), Riccardo SPEZIA (LCT), Simon HUPPERT (INSP)


0.16
0.12
0.08
0.04
0.00
Energy (a.u)
−0.6
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
Reaction Coordinate (a.u)
S
N
O
H


0.16
0.12
0.08
0.04
0.00
Energy (a.u)
−0.6
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
Reaction Coordinate (a.u)
S
N
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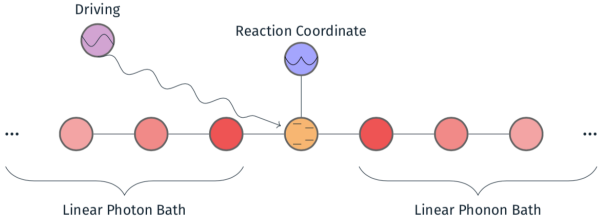
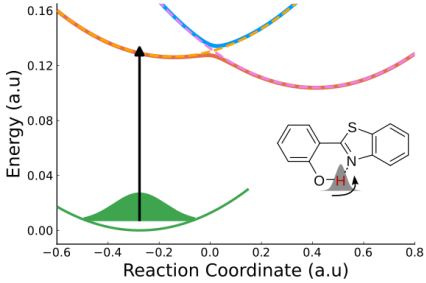
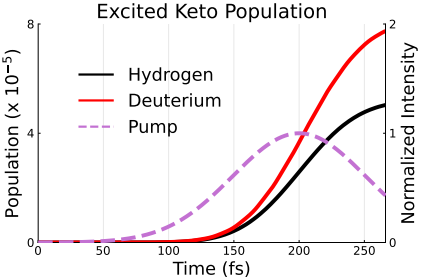
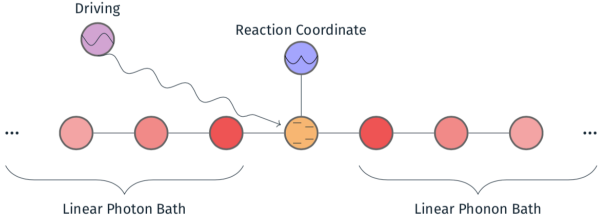
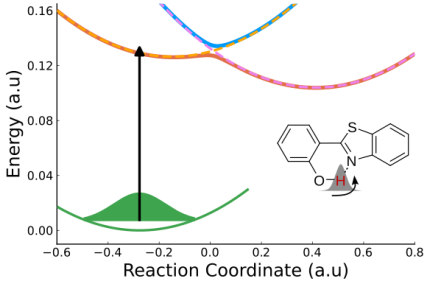
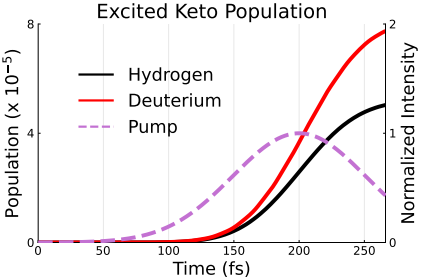

Driving
Reaction Coordinate
Linear Photon Bath
Linear Phonon Bath


Energy (a.u)
Reaction Coordinate (a.u)
S
N
O
H


Excited Keto Population
Hydrogen
Deuterium
Pump
Population (x 10⁻⁵)
Normalized Intensity
Time (fs)


Driving
Reaction Coordinate
Linear Photon Bath
Linear Phonon Bath


Energy (a.u)
Reaction Coordinate (a.u)
S
N
O
H


Excited Keto Population
Hydrogen
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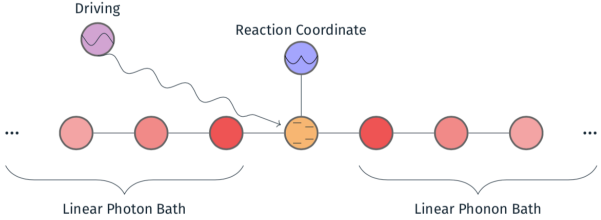
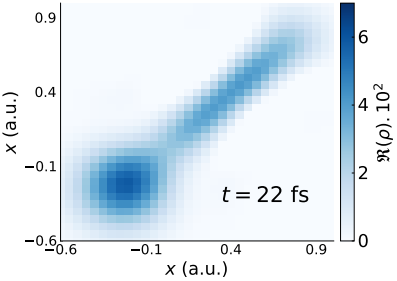
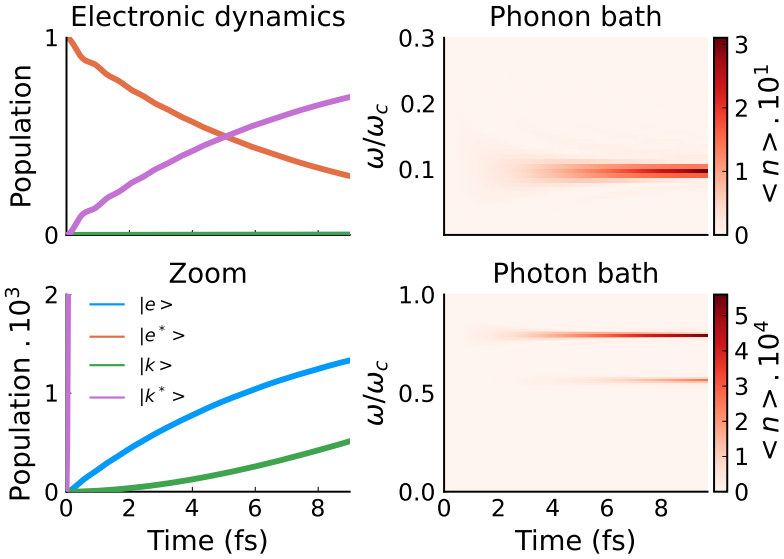
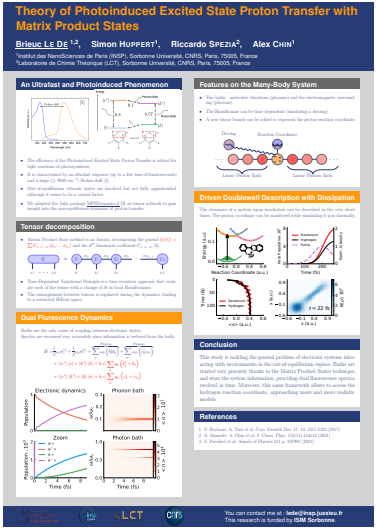
Population (x 10⁻⁵)
Normalized Intensity
Time (fs)


Driving
Reaction Coordinate
Linear Photon Bath
Linear Phonon Bath


t = 22 fs
x (a.u.)
x (a.u.)
ℜ(ρ). 10²


Electronic dynamics
Population
1
0
Phonon bath
ω/ω_c
0.3
0.2
0.1
$< n > . 10^1$
3
2
1
0
Zoom
Population . 10^3
2
1
0
$|e>$
$|e^*>$
$|k>$
$|k^*>$
0
2
4
6
8
Time (fs)
Photon bath
ω/ω_c
1.0
0.5
0.0
$< n > . 10^4$
5
4
3
2
1
0
0
2
4
6
8
Time (fs)



Feel free to come to my poster :)