Using quantum dynamics to reveal properties of excited states

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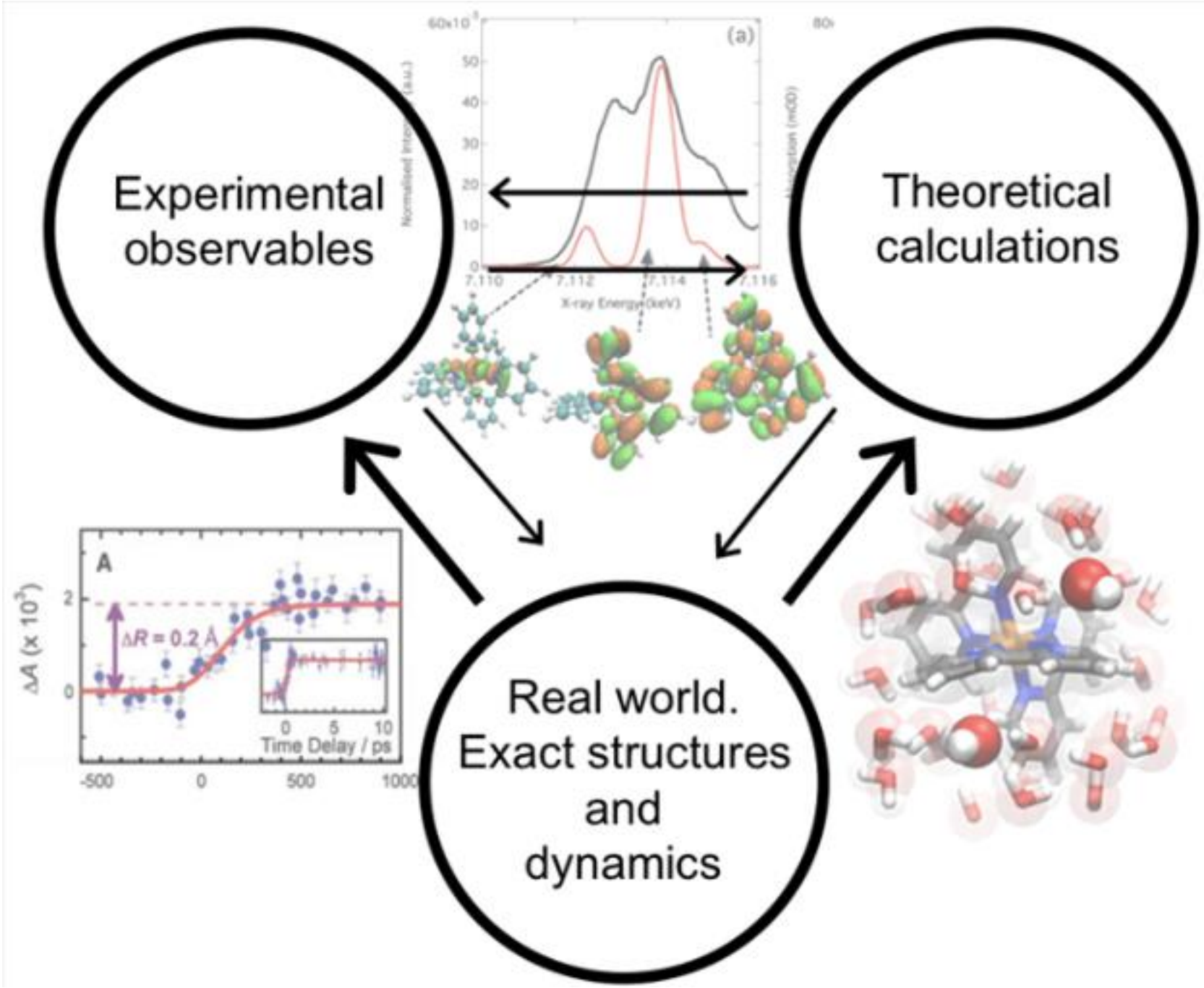
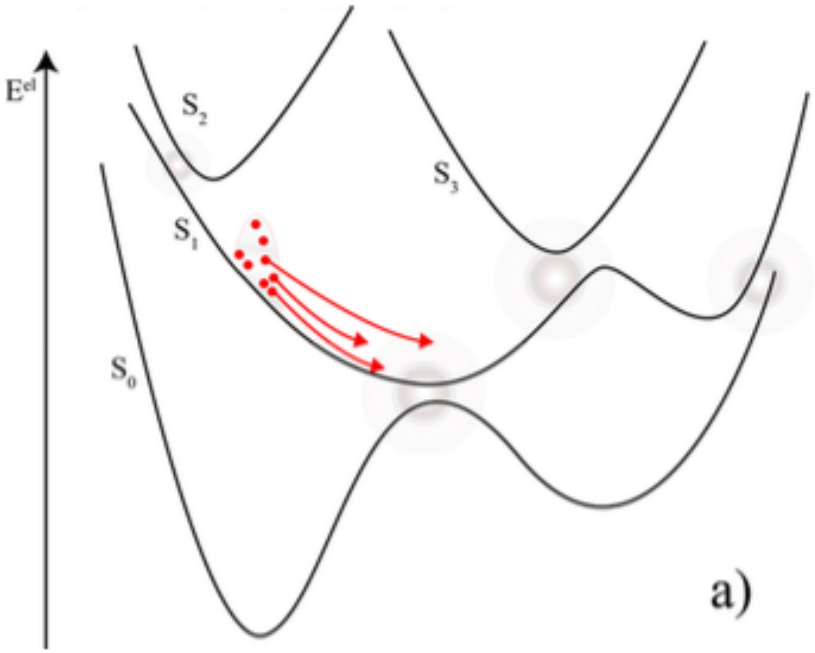
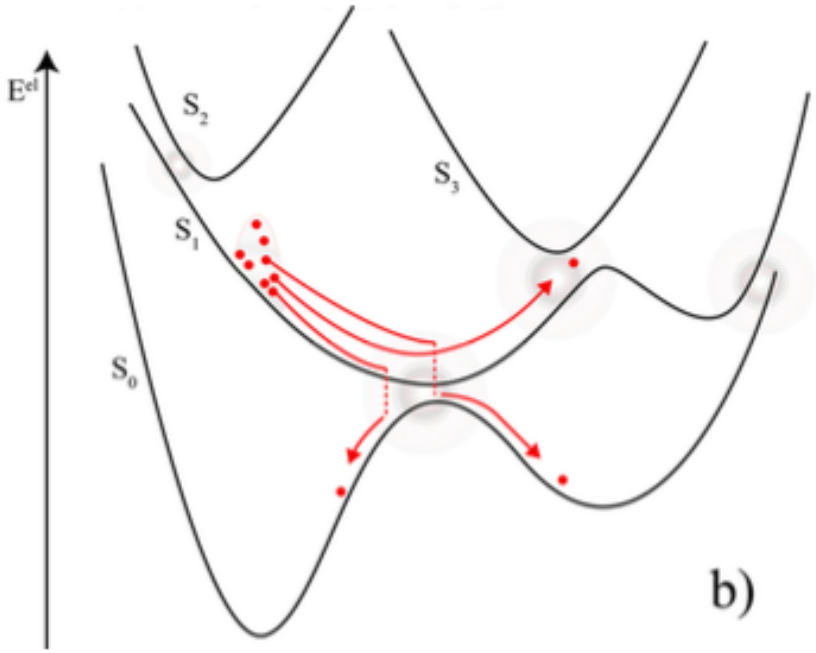
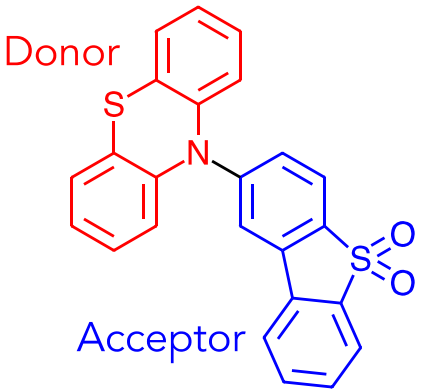
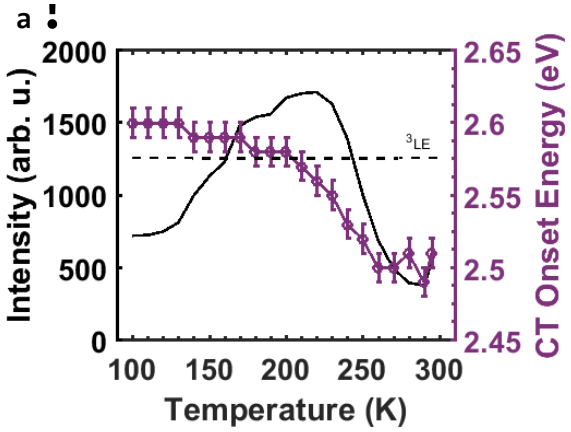

Experimental observables
Theoretical calculations
Real world. Exact structures and dynamics
(a)
X-ray Energy (keV)
A
ΔR = 0.2 Å
ΔA (x 10³)
Time Delay / ps

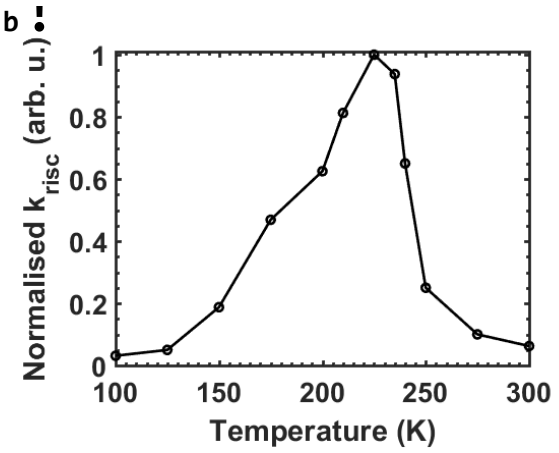
Excited State Dynamics



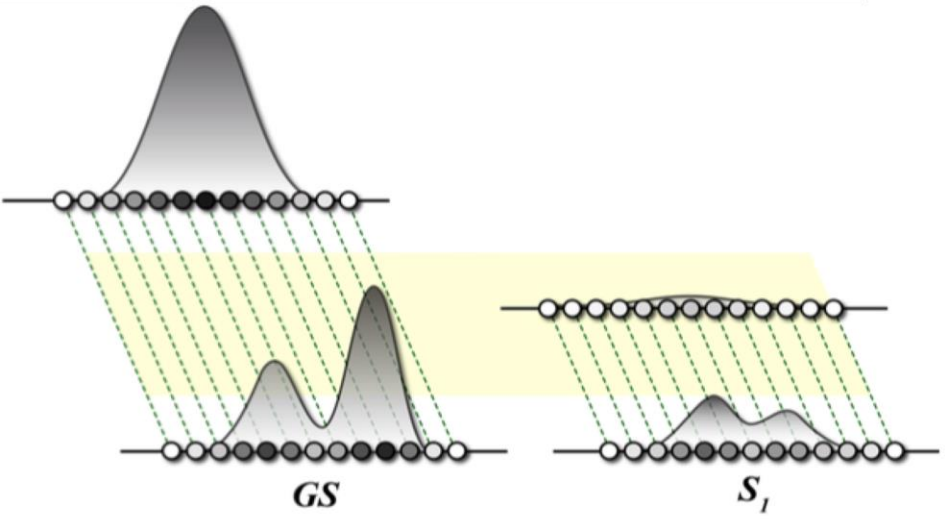


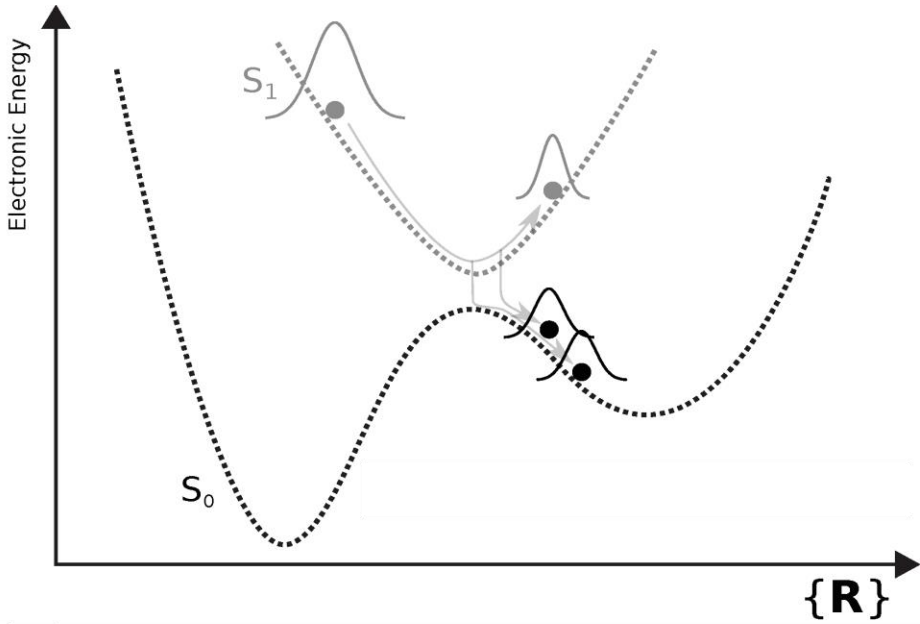


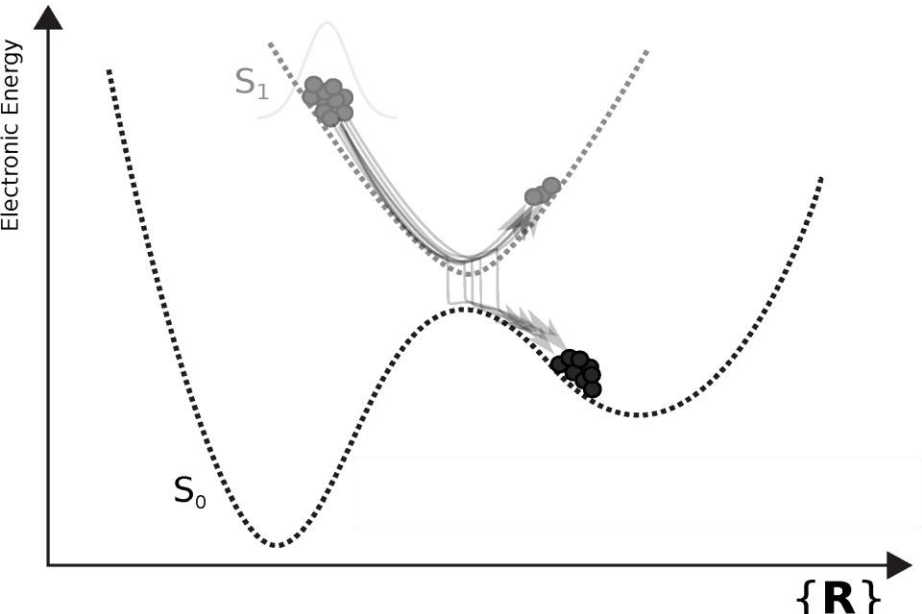


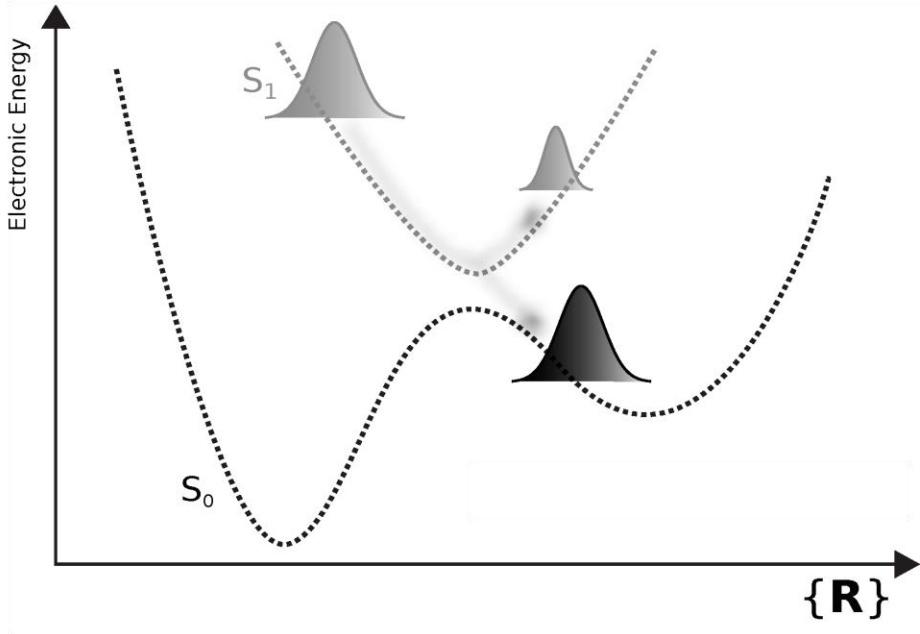


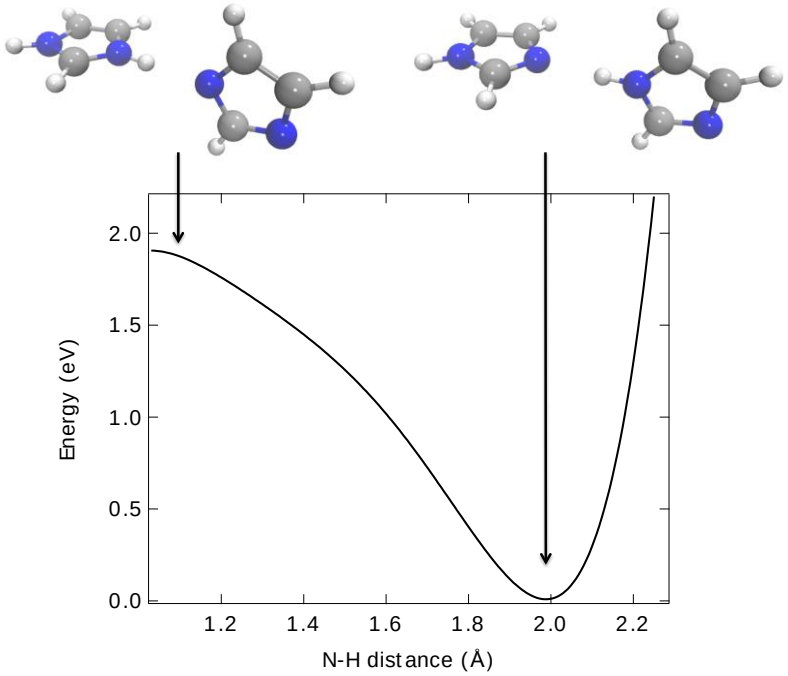
Methods for Dynamics

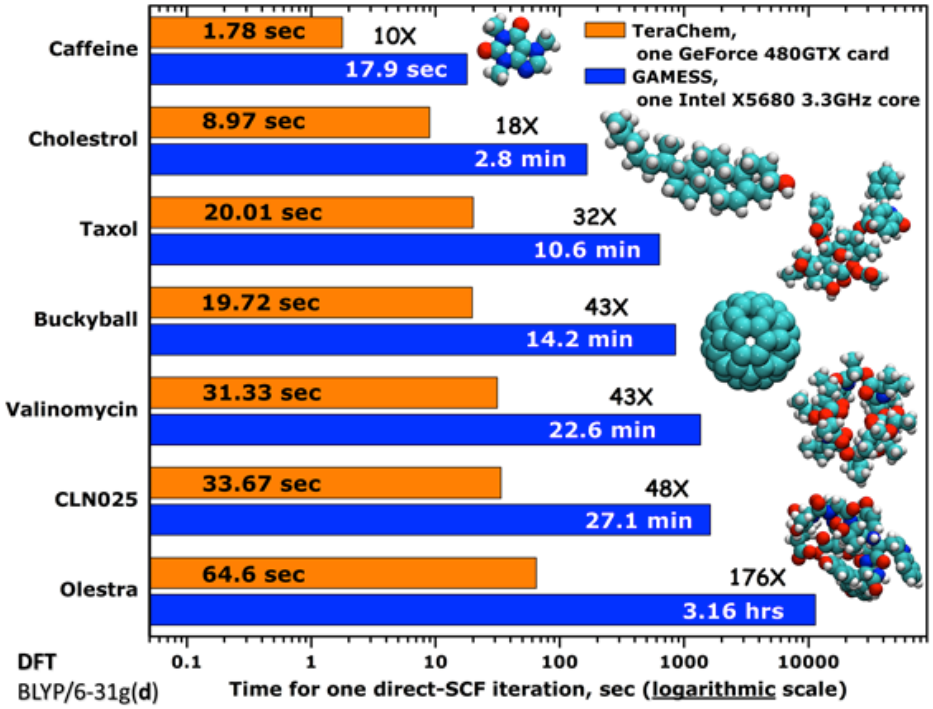


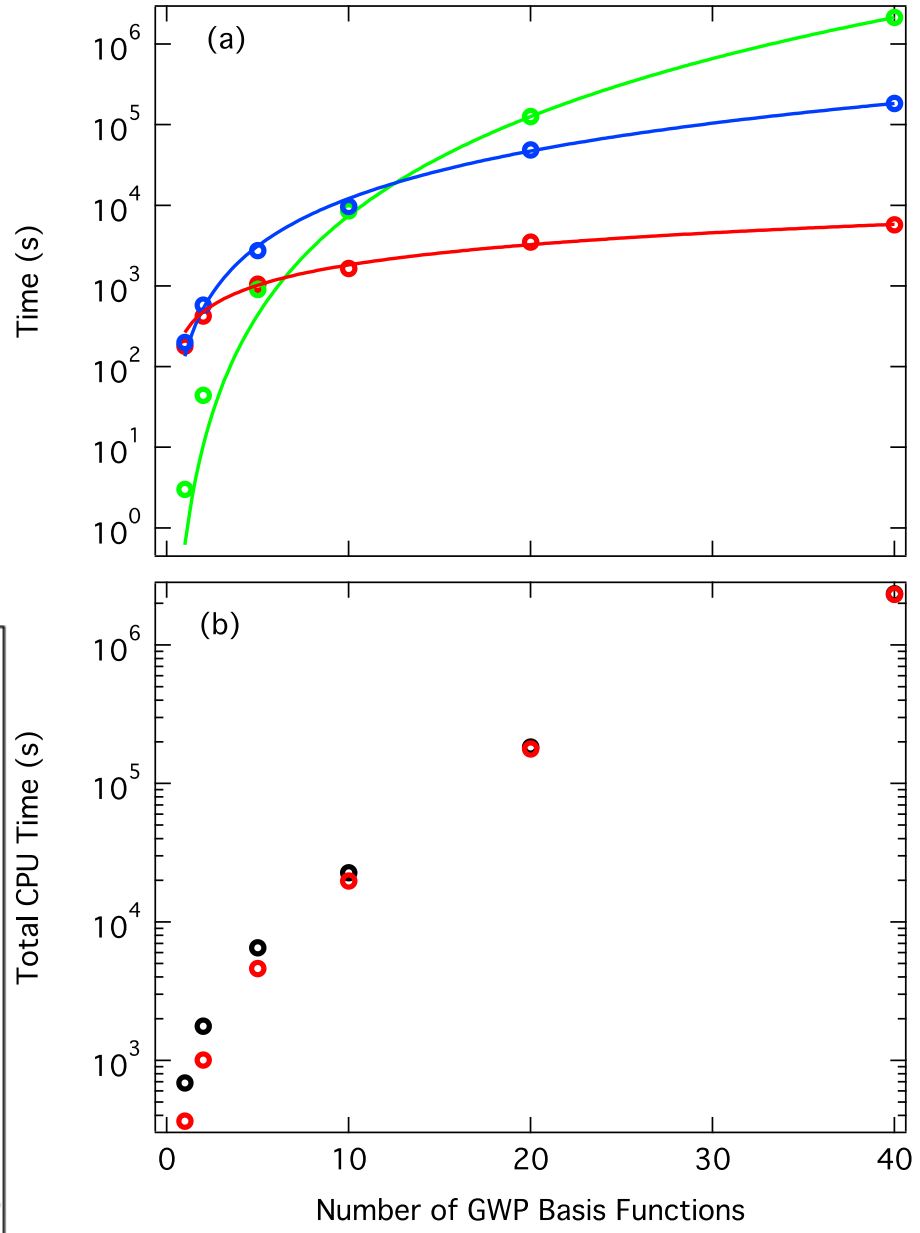


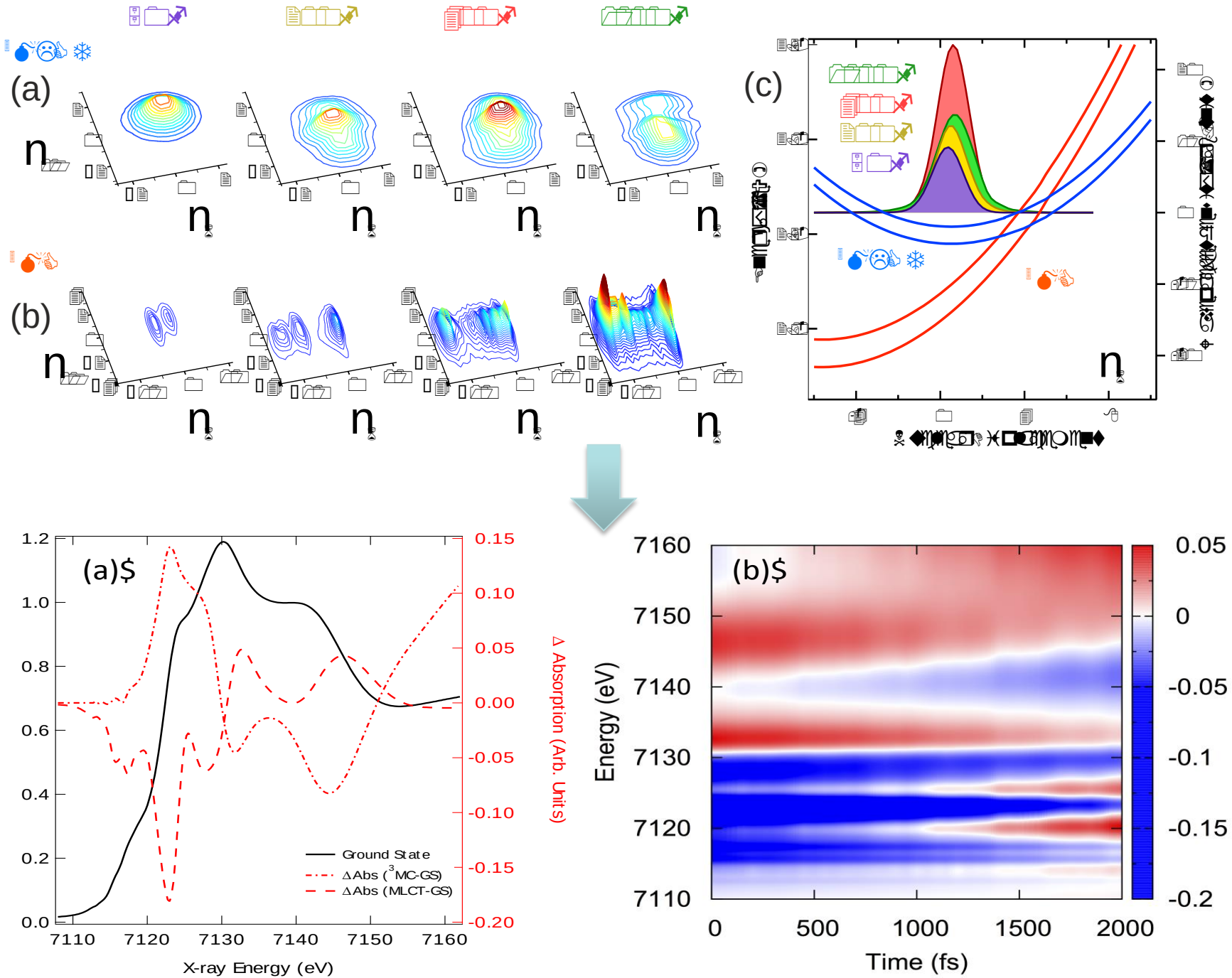





Energy (eV)
N-H distance (Å)


Caffeine
1.78 sec
10X
17.9 sec
Cholestrol
8.97 sec
18X
2.8 min
Taxol
20.01 sec
32X
10.6 min
Buckyball
19.72 sec
43X
14.2 min
Valinomycin
31.33 sec
43X
22.6 min
CLN025
33.67 sec
48X
27.1 min
Olestra
64.6 sec
176X
3.16 hrs
TeraChem, one GeForce 480GTX card
GAMESS, one Intel X5680 3.3GHz core
DFT
BLYP/6-31g(d)
Time for one direct-SCF iteration, sec (logarithmic scale)


(a)
(b)
Time (s)
Total CPU Time (s)
Number of GWP Basis Functions


(a)
n
n
n
n
n
(b)
n
n
n
n
n
(c)
n
(a)$
Absorption (Arb. Units)
Δ Absorption (Arb. Units)
X-ray Energy (eV)
Ground State
ΔAbs (3MC-GS)
ΔAbs (MLCT-GS)
(b)$
Energy (eV)
Time (fs)

Summary

Main interest/Skills

- Non-equilibrium dynamics with quantum nuclear effects.
- Excited state dynamics.
- Quantum nuclear dynamics.
- Spectroscopy, especially time-resolved and core-level.
- Collaborations with experimental groups.