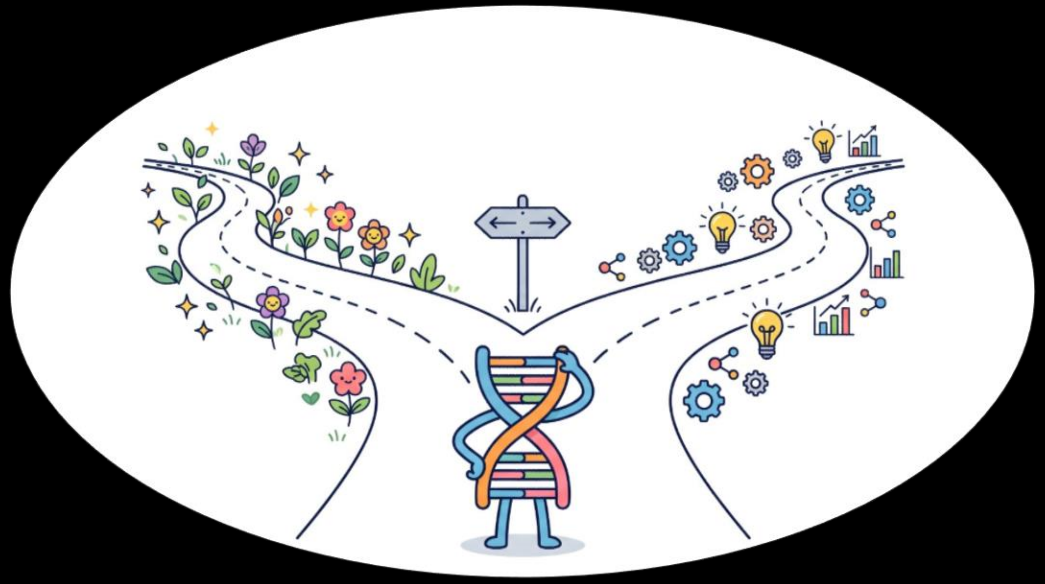
The Hidden Routes of DNA Photostability

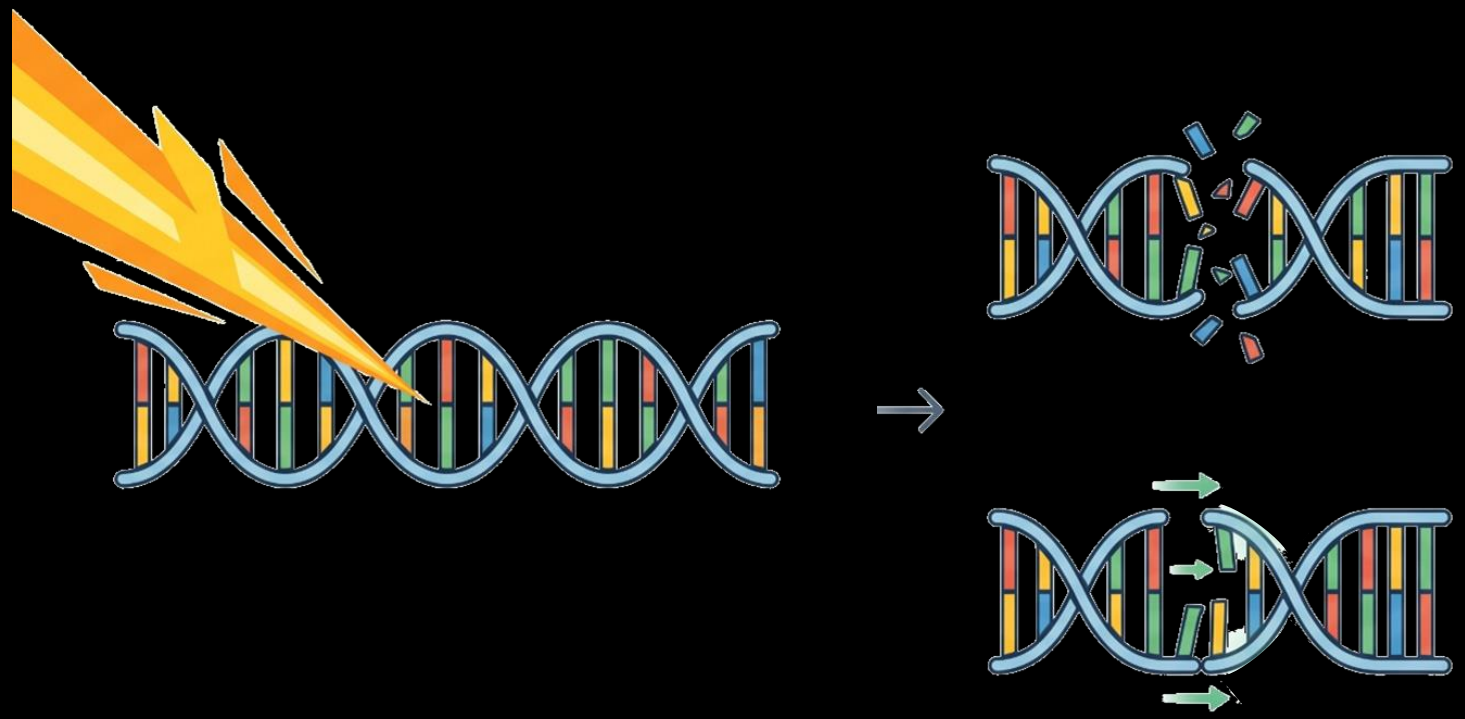
Juliana de Abrantes, Josene Toldo, Mario Barbatti, Marco Sacchi



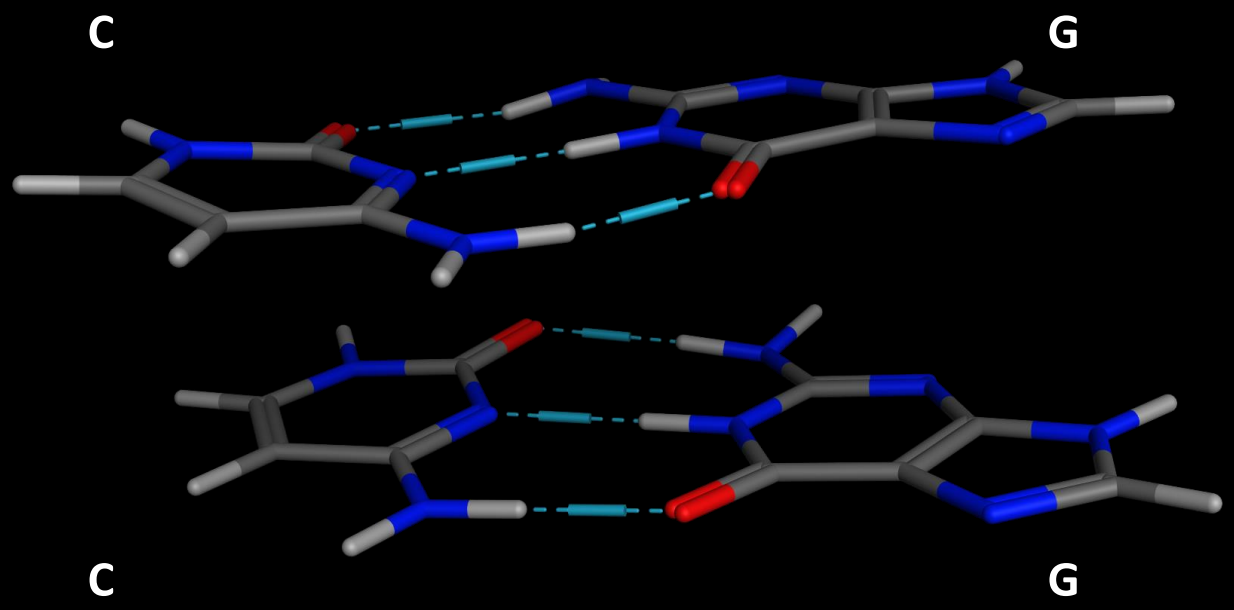
J. Phys. Chem. Lett. 2026, 17, 5709−5717

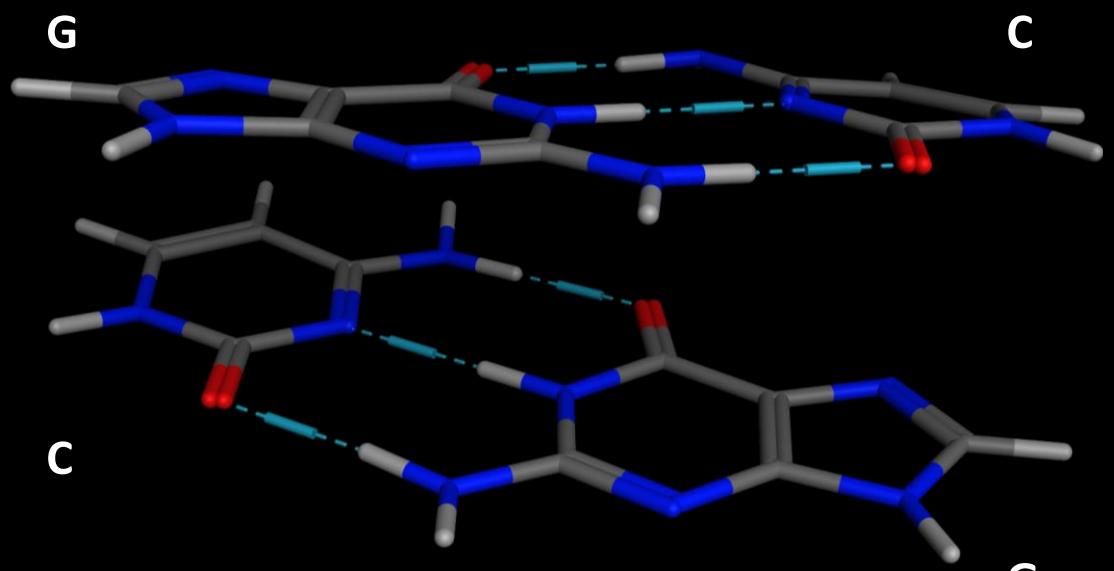
UNIVERSITY OF SURREY

Photodamage vs Photostability



System

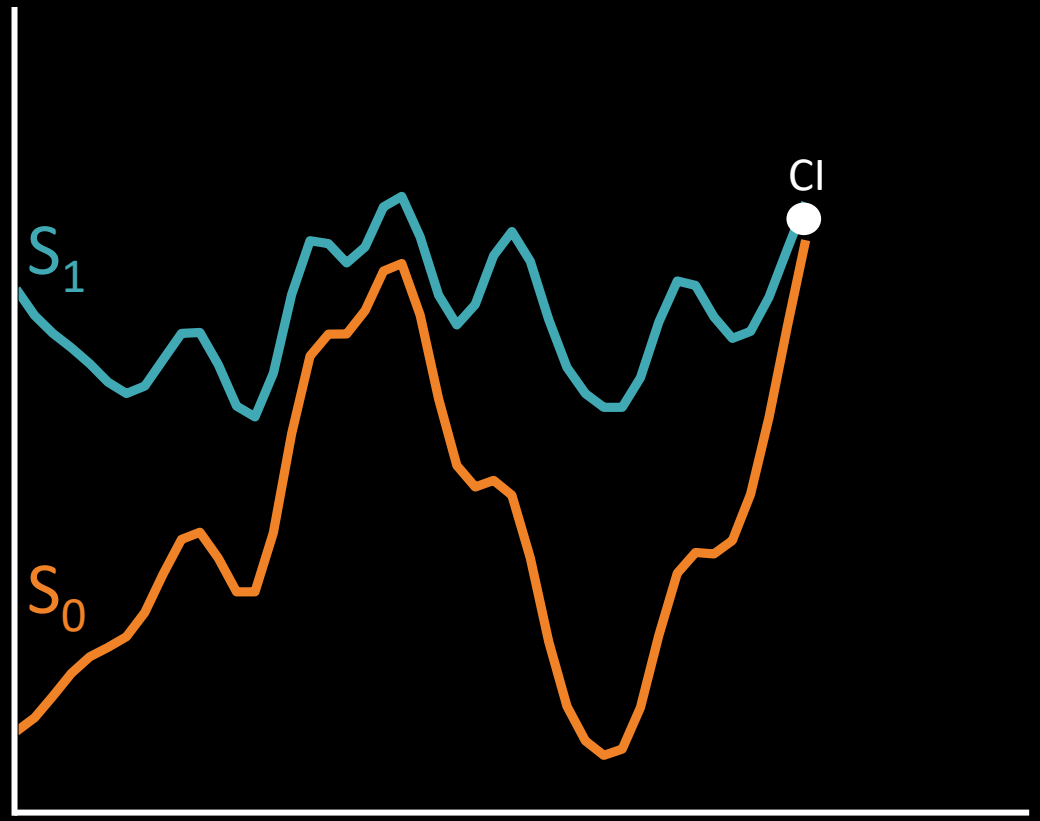




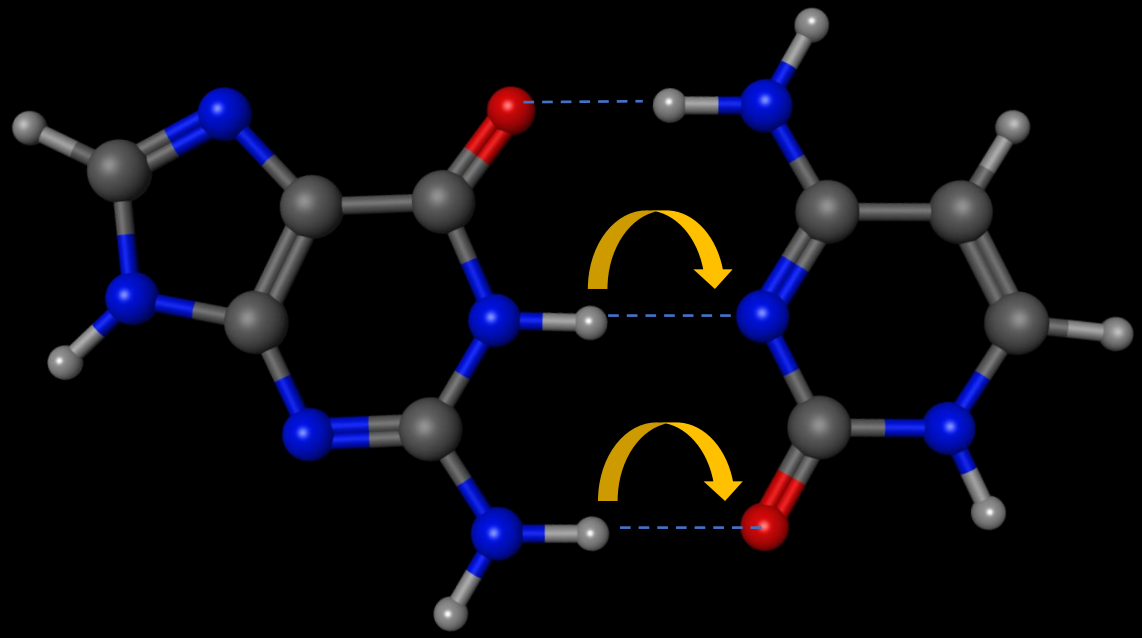
Method

- Surface hopping (DC-FSSH)
- 100 trajectories

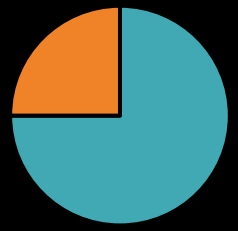
- TD-DFT
- CAM-B3LYP + D4, 6-31G*

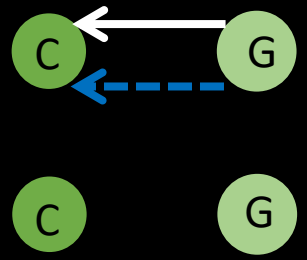


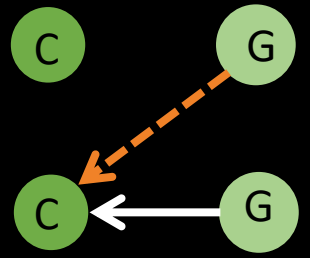
Decay mechanism

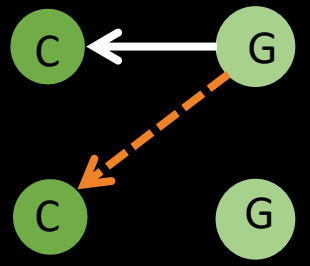


ESHT vs PCET

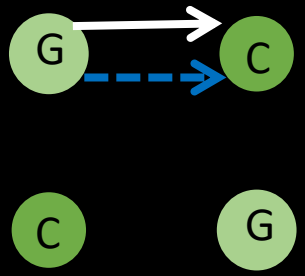


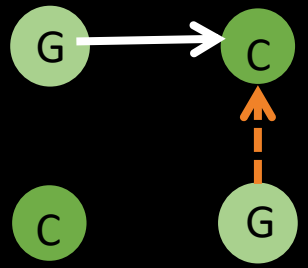


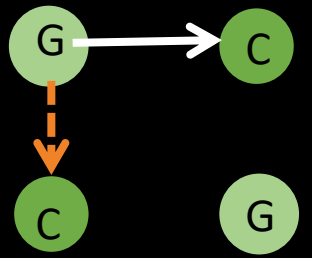




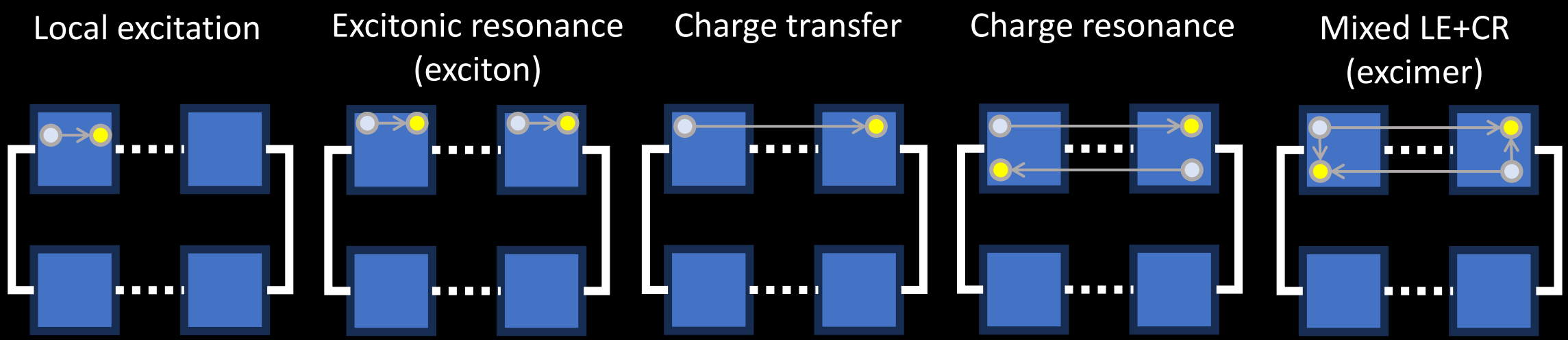






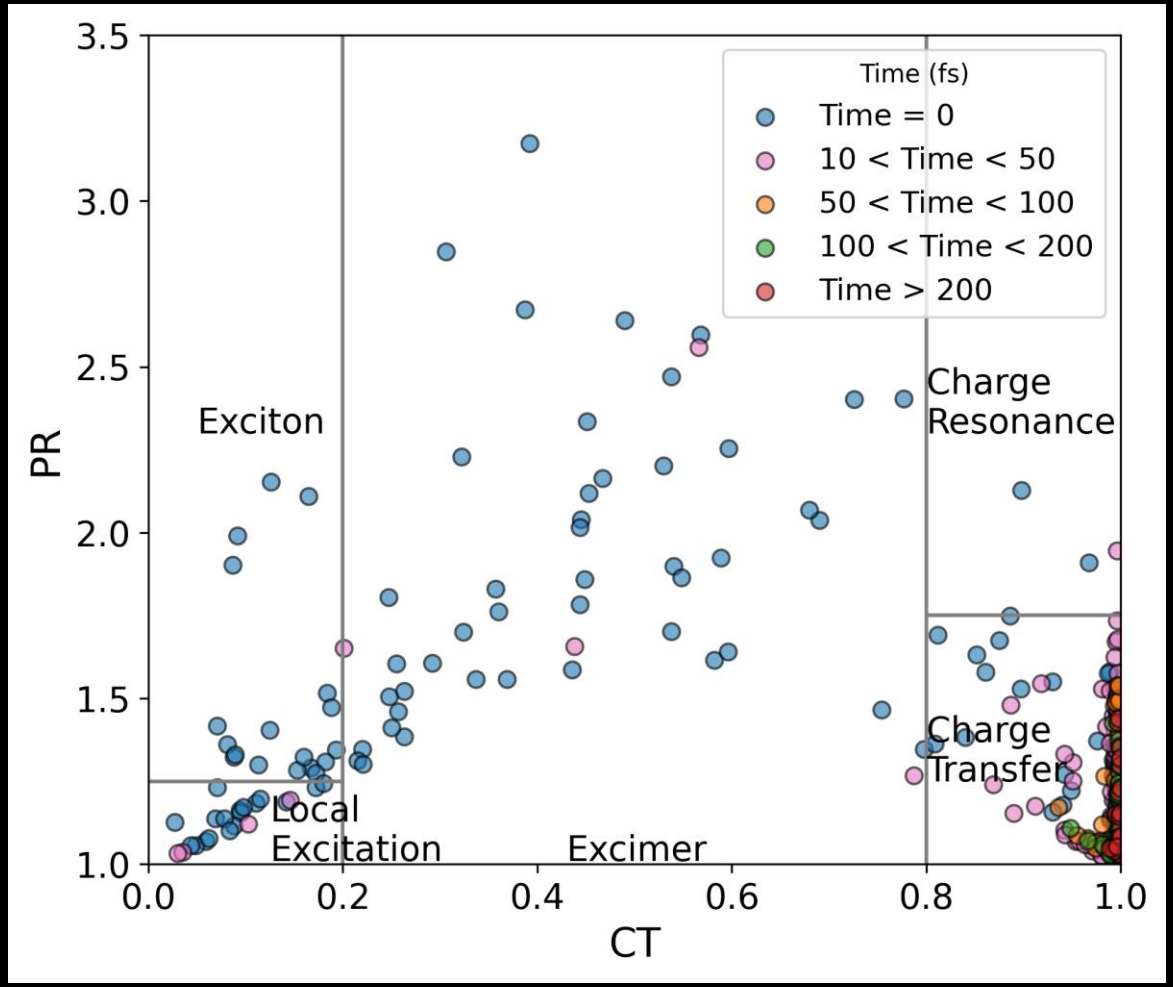


Classification of excitation

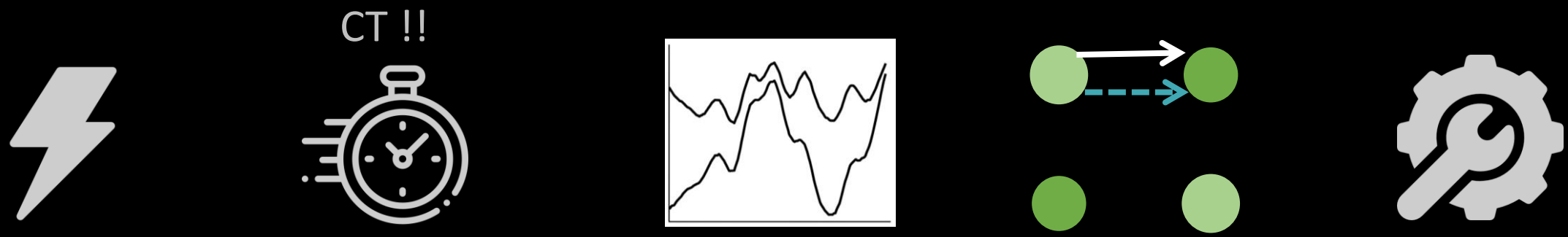


hole
electron

1-TDM analysis



Mechanistic picture



Conclusions



ES relaxation in stacked GC systems is CT driven



N-N PT is the dominant identified decay channel



Electron-transfer pathways are diverse and sequence-dependent



DNA photostability emerges from coupled electron and proton motion

Thank you

juliana.g.abrantes@gmail.com







