Investigating Photodynamics of Nucleobase–Water Systems

Haseena Sheik,[a] **Luca Grisanti**,[b] **Tea Ostojić**,[c] **Chaiyaporn Lakmuang**,[a] **Barbara Rossi**[c] **and Antonio Prlj**[a]

hsheik@irb.hr

[a]*Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia*
[b]*National Research Council, CNR-IOM, Via Bonomea 265, 34136 Trieste, Italy*
[c]*Elettra Sincrotrone Trieste, Strada Statale 14 km 163.5, 34149 Trieste, Italy*

This study examines the photodynamics of weakly bound hydrogen-bonded molecular systems, with a primary focus on developing a pragmatic computational protocol that incorporates flexibility and quantum distributions of initial conditions for nonadiabatic dynamics. As a case study, the photodynamics of 2,6-diaminopurine nucleobase-water clusters has been investigated in both its 7H and 9H tautomeric forms. Simulations are performed in vacuum and aqueous solution (implicit water clusters) using DFT/TDDFT electronic structure. Our results highlight the influence of solvation on the excited-state dynamics and the role of conical intersections in system relaxation back to the ground state. This study provides deeper insights into the photophysics/photochemistry of purine derivatives and their implications for photostability in biological and biomimetic systems.

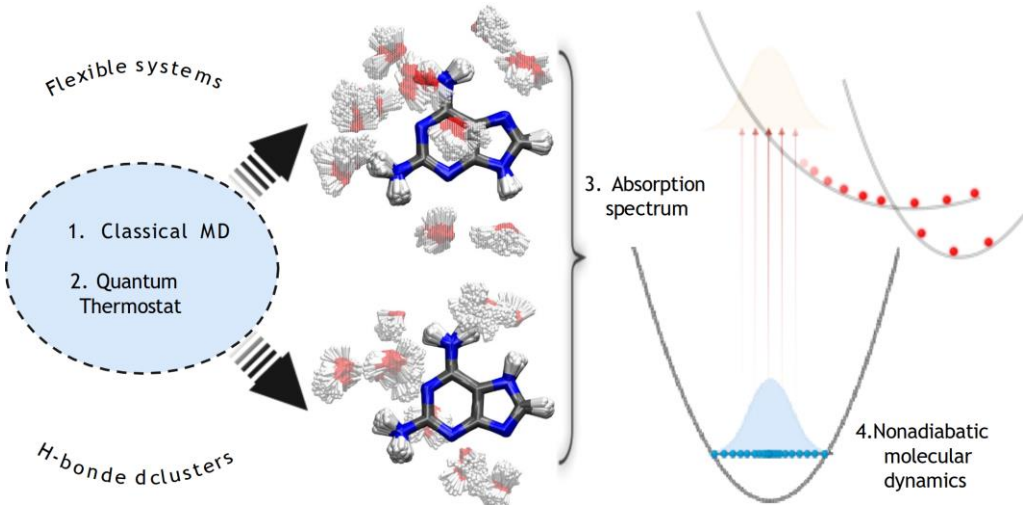

Figure 1. Schematic representation of workflow for simulating ultrafast relaxation of 2,6-diaminopurine nucleobase-water clusters

References:

[1] H. Sheik, L. Grisanti, T. Ostojić, C. Lakmuang, B. Rossi, A. Prlj, *Phys. Chem. Chem. Phys.* **27** (2025) 18112-18115.