

An Ab Initio Microscope: Molecular Contributions to the Femtosecond Time-Dependent Fluorescence Shift of a Reichardt-Type Dye

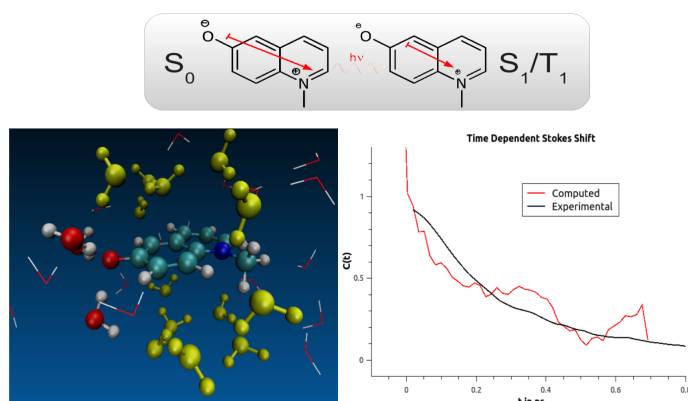
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The molecular probe N-methyl-6-quinolone (MQ) gives spectroscopic access to its local environment.[1] Its experimentally observed time-dependent Stokes shift can be explained by molecular dynamics simulations in combination with DFT calculations. Decomposition of the MD trajectories shows that an important contribution to the time-dependent Stokes shift originates from a group of water molecules that strongly interact with the molecular dipole of MQ.[2]



The approach we have been taken to simulating the excited state solvation dynamics[3] is currently being applied to excited state proton transfer.

[1] Pérez-Lustres, J. L., Mosquera, M., Senyushkina, T., Kovalenko, S. A., Flasche, W., Ernsting, N. P. *Angew. Chem. Intl. Ed.*, 44:5635-5639, **2005**.

[2] C. Allolio, M. Sajadi, N.P. Ernsting and D. Sebastiani *Angew. Chem. Intl. Ed.*, 52:1813-1816, **2013**.

[3] C. Allolio and D. Sebastiani: *Phys. Chem. Chem. Phys.*, 13:16395-16403, **2011**.