A DFT/TDDFT STUDY OF KETOCYANINE DYE INTERACTIONS WITH Li^+ AND Mg^{2+}

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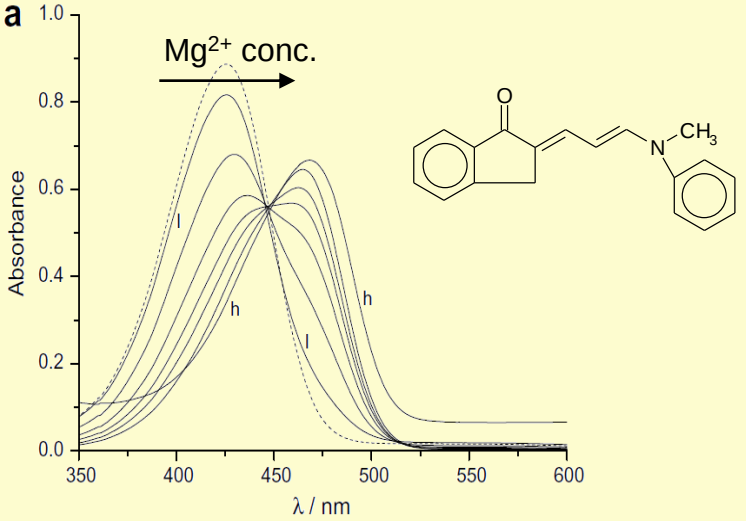
Motivation:

- TDDFT is a standard tool in studies of excited states in organic molecules
- less attention has been paid to the complexes



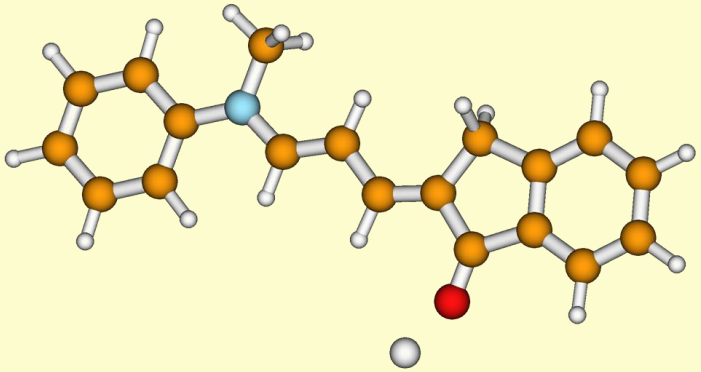
J.K.Basu, M. Shannigrahi, S. Bagchi, *Chem. Phys. Lett.* **441** (2007) 336

Recently, experimental data became available for ketocyanine dyes complexed with Li^+ or Mg^{2+}

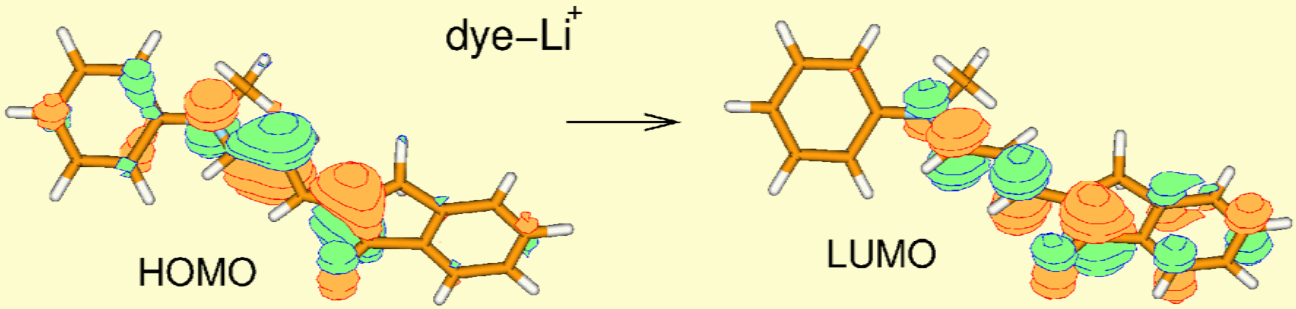
Opportunity to check the methodology

Calculations have been performed in the ACK Cyfronet Computing Centre (grant no. MNiSW/IBM_BC_HS21/UJ/02/2009)

DFT geometry optimizations and
binding energy calculations
in vacuum and in the solvent (PCM)



TDDFT calculations for the S0 → S1 transition



Conclusions

Accounting for solvent effects necessary for reasonable reproduction of spectral shifts

The best agreement between calculated and observed shifts in absorption spectra obtained for hybrid B3LYP functional