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Visual readout – enabled systems Merocianine – β-Cyclodextrin complexes as photo controlled material actuators

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INTRODUCTION & AIM

The interaction between beta-cyclodextrin (β-CD) and the merocyanine form of 4-[(2E)-1,1-dimethyl-2-({[(1Z)-2-oxo-1,2-dihydronaphthalen-1-ylidene]amino}methylidene)-1H,2H,3H-benzo[e]indol-3-yl]butane-1-sulfonic acid (MC) was investigated to elucidate host-guest complexation dynamics and stability, in order to develop applications such as photoswitches for imaging and therapy. These are possible do to MC's absorption changes with isomerization therefore, the β-CD environment can provide a consistent, water-compatible platform and potentially targetable coatings. β-CD is a cyclic oligosaccharide, that is well known for their ability to form "inclusion complexes" with other molecules, changing the properties of the guest molecule upon binding.

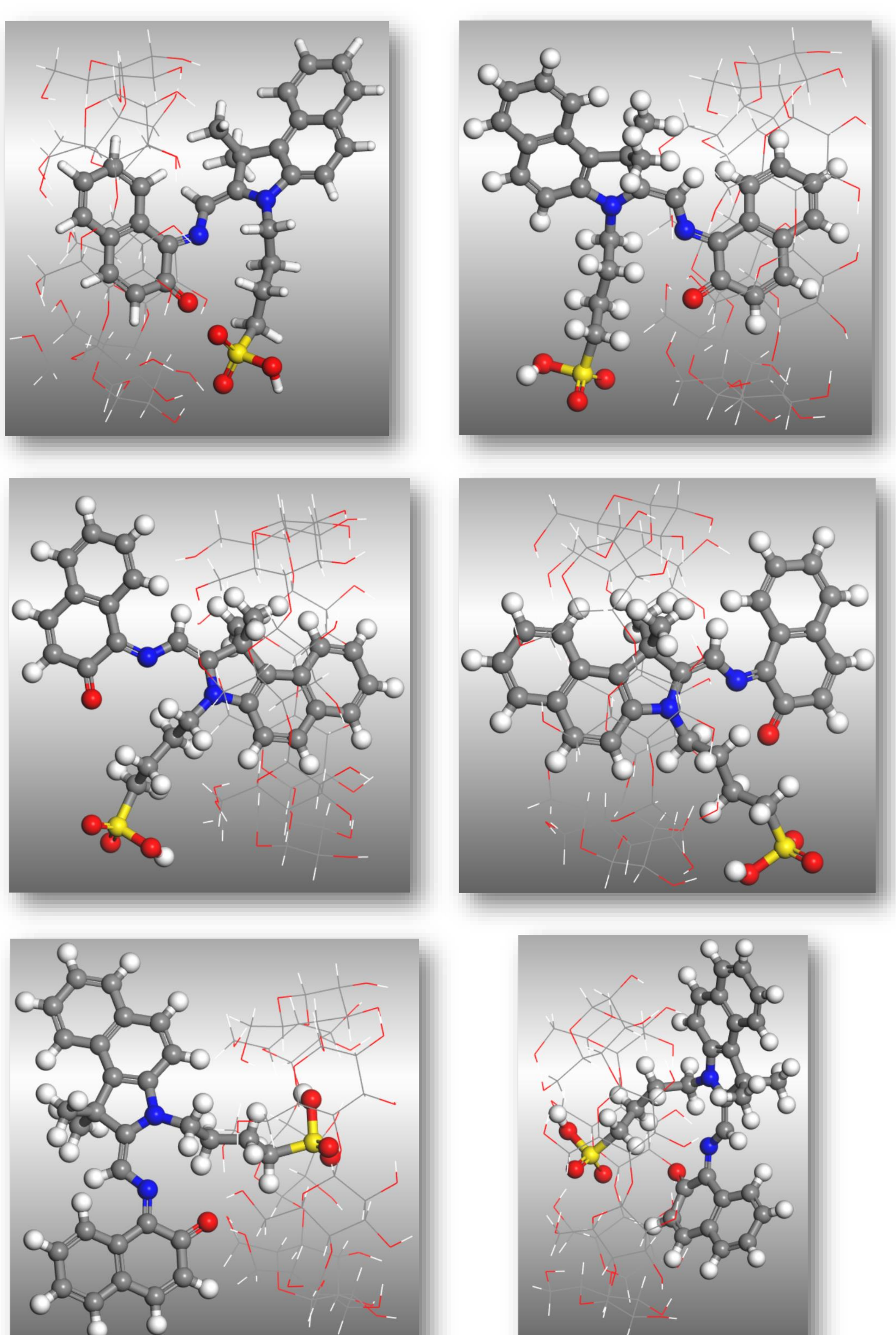
Aim:

- DFT calculations for investigation of MC in presence of β-CD;
- Investigation of the spectral propertiesof MC/β-CD system;

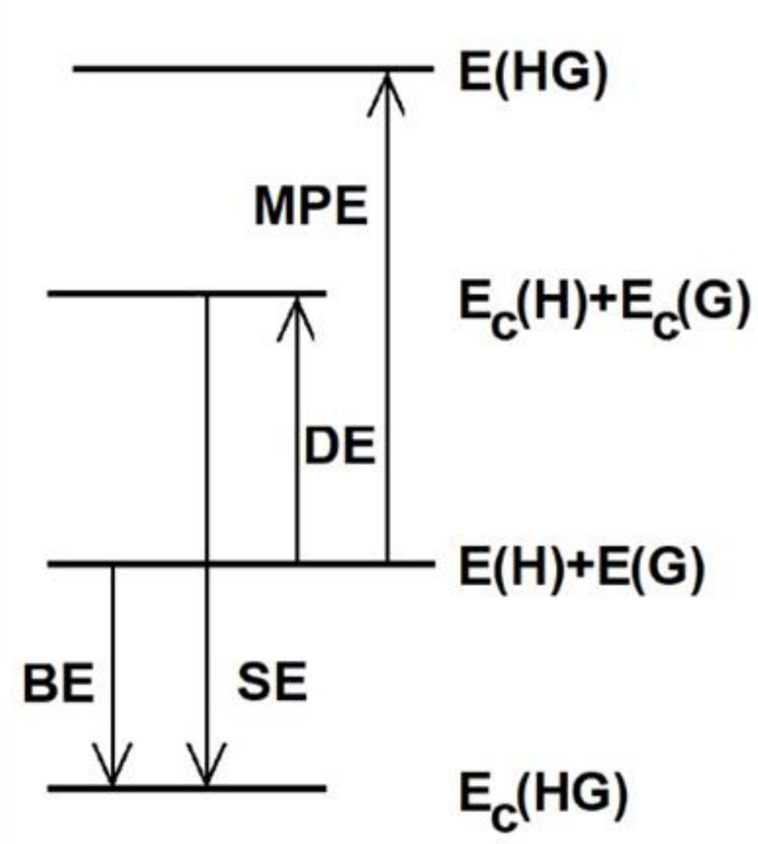
METHOD

- DFT (Density Functional Theory) calculations was used to calculate various properties of MC, including electronic structure, energies, and geometries. Functional GGA/PW91; OBS correction was used.
- UV-Vis spectra were carried out on a Carry 300 Bio spectrophotometer equipped with a temperature controlled cell holder in the range of 200 – 800 nm using 1x1x4 - cm micro quartz cells with teflon stopper.

RESULTS & DISCUSSION

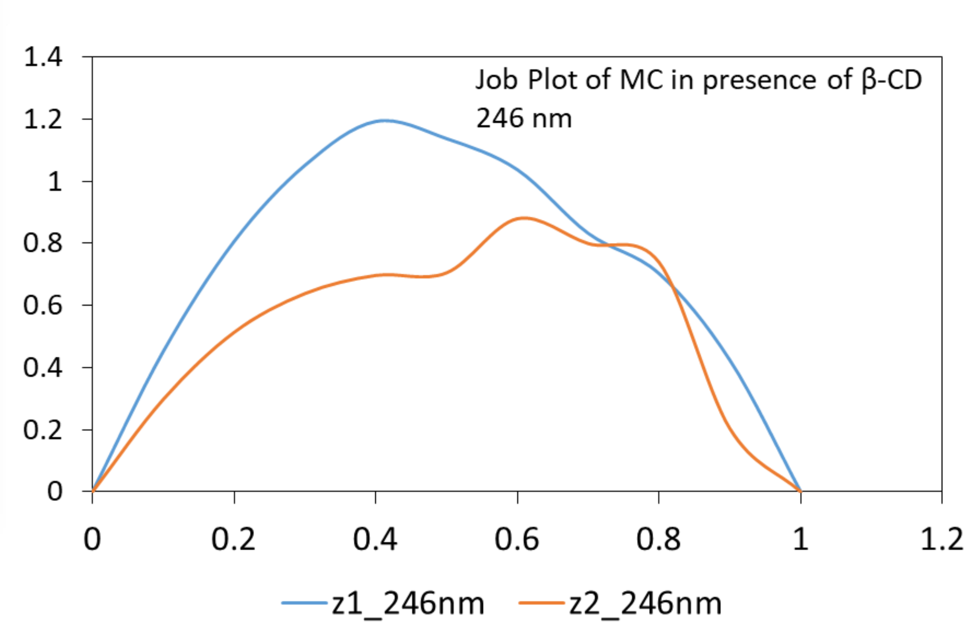


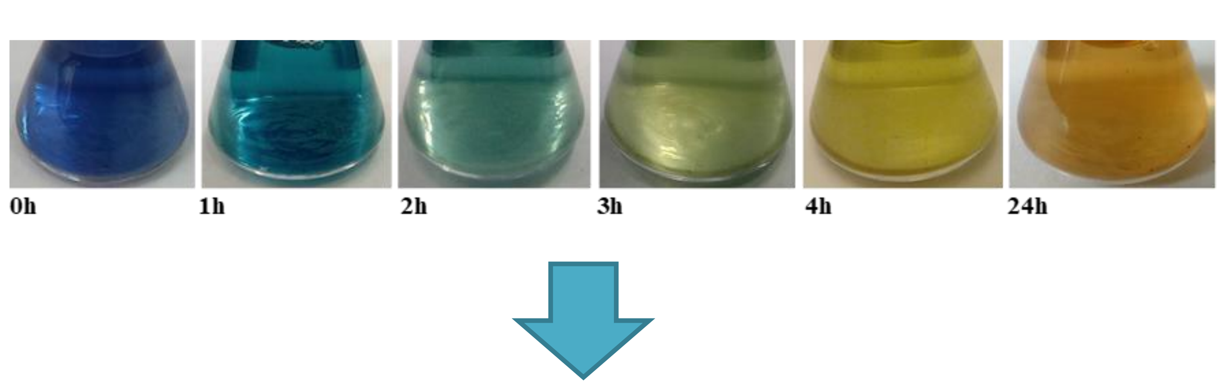
Spatial representation of the equilibrium geometries of three types of 1:1 host-guest assemblies - side view (primary hydroxyl rim of CD positioned to left side) of MC/ β-CD. Type one of the 1:1 complex is by positioning the function group (each of the function groups: naphtooxazine, indole and butyl-1-sulfonate) of the MC toward the wider rim of the CD (left side of each panel) and type two is for the function group of the MC toward the narrow rim of the CD molecule (right side of each panel). The color correspondence is: blue for N atoms, grey for C atoms, yellow for H atoms, and red for O atoms.



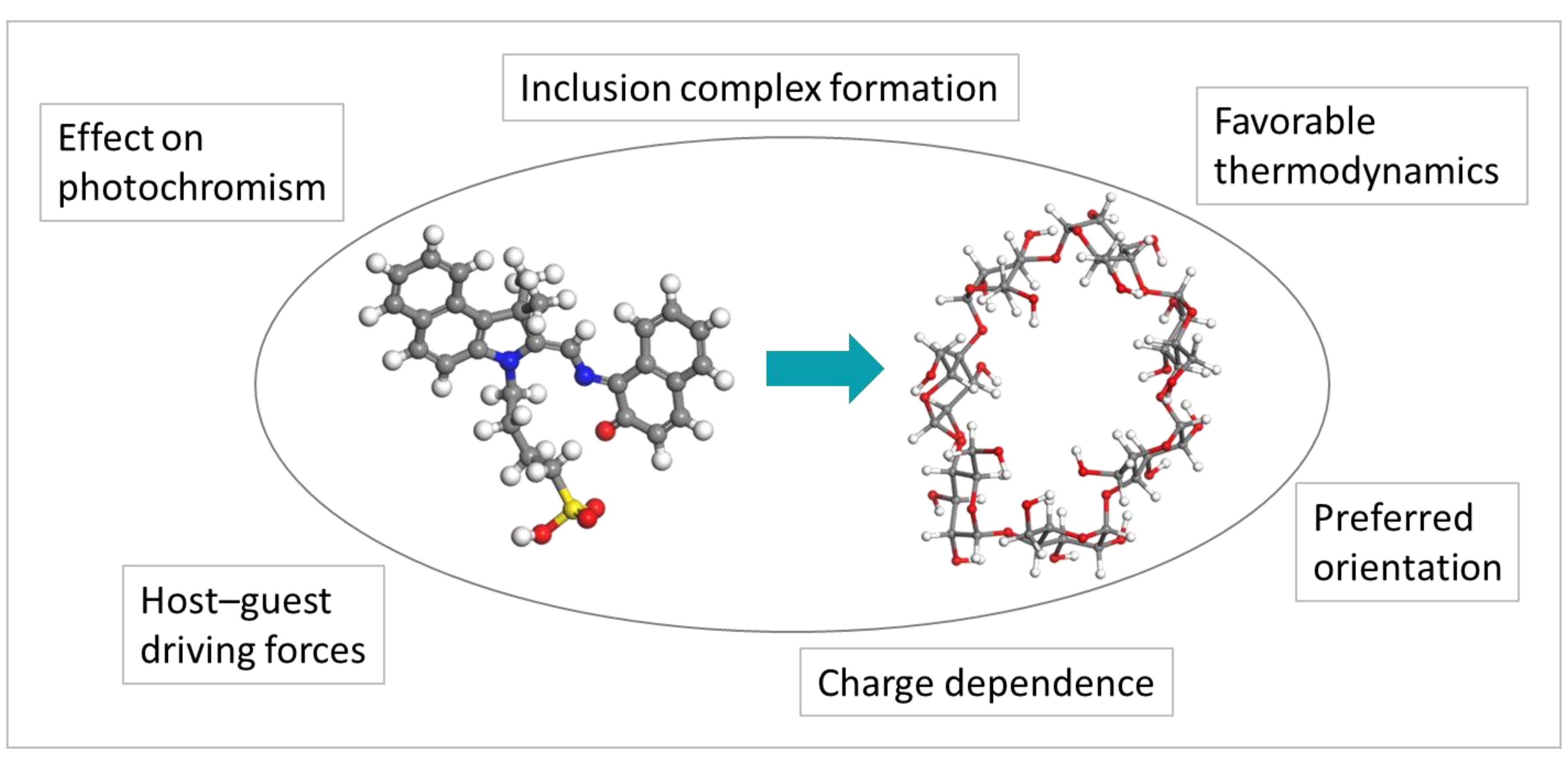
$$MPE(HG) = E(HG) - E(H) - E(G)$$
$$DE(HG) = E(HG) - E_c(HG)$$
$$BE(HG) = E_c(HG) - E(H) - E(G)$$
$$SE = E_c(HG) - E_c(H) - E_c(G) = BE - DE$$
$$SE = - MPE$$

The various energies involved in computing of the MPE, SE, BE, DE quantities: E(HG) – the energy of the host – guest assembly, H and G molecules having optimized geometries; Ec(HG) – the energy of the inclusion complex; E(H) + E(G) – the sum of the energies of the optimized geometries of the host and guest molecules, Ec(H) + Ec(G) – the sum of the energies of the H and G molecules. The "c" index refer to molecules or assemblies which have the geometry from the complex. The energies without the "c" index refer to molecules that have optimized geometries.





After irradiation produces MC, β-CD host retain MC, and this slows the thermal back-reaction trans-MCH^+ → SP, compared to water.



CONCLUSION

MC interacts with β-CD primarily through noncovalent host–guest inclusion, driven by hydrophobic effects, van der Waals contacts, and hydrogen bonding. Binding alters electronic structure, photochemical behavior, and stability of the merocyanine, with strong dependence on merocyanine protonation and β-CD substitution pattern.