Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Ultrafast Multiexponential Electron Injection Dynamics at dye and ZnO QD Interface: A Combined Spectroscopic and First Principles Study

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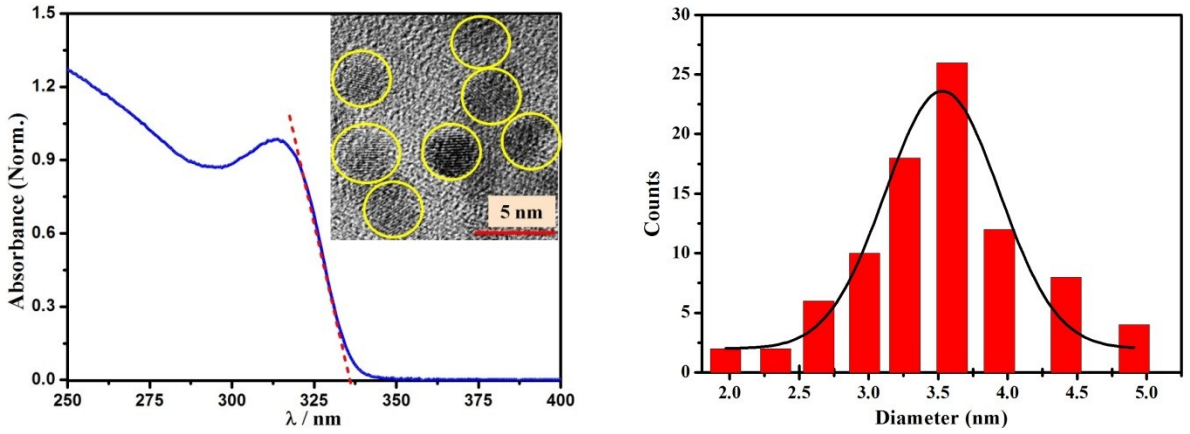
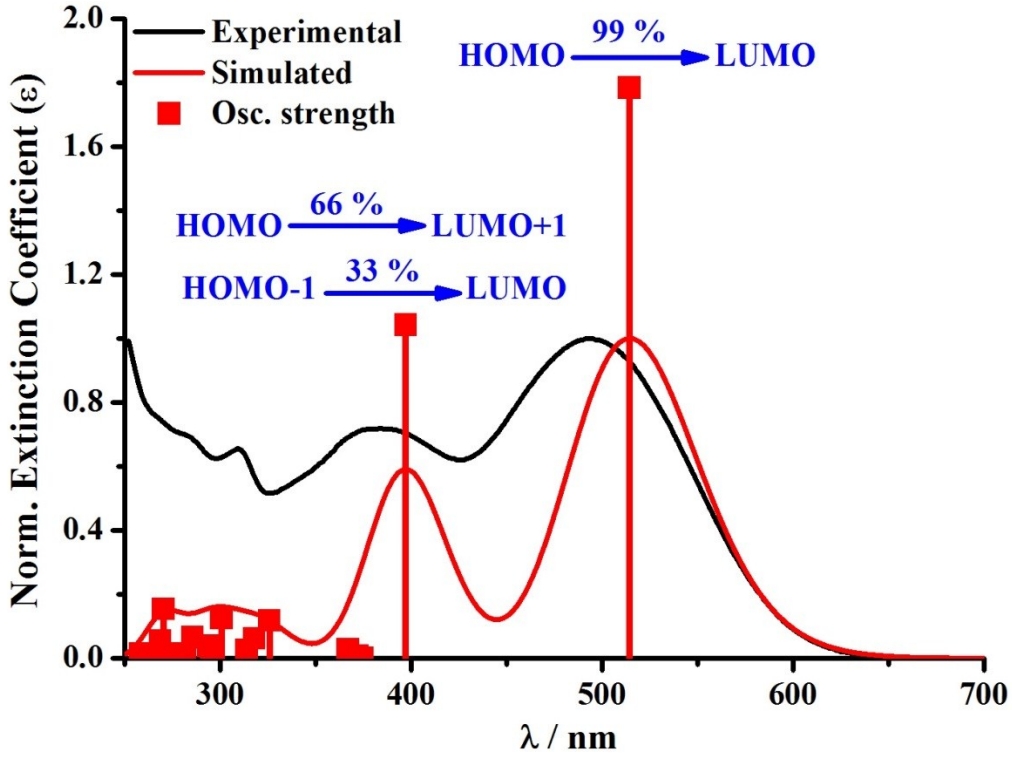


(a) **(b)**

Figure S1. (a) UV-vis absorption spectra of ZnO QDs showing a sharp excitonic peak at 314 nm (3.95 eV), where inset depicts high resolution TEM images of ZnO QDs. **(b)** Histogram for the particle size distribution.



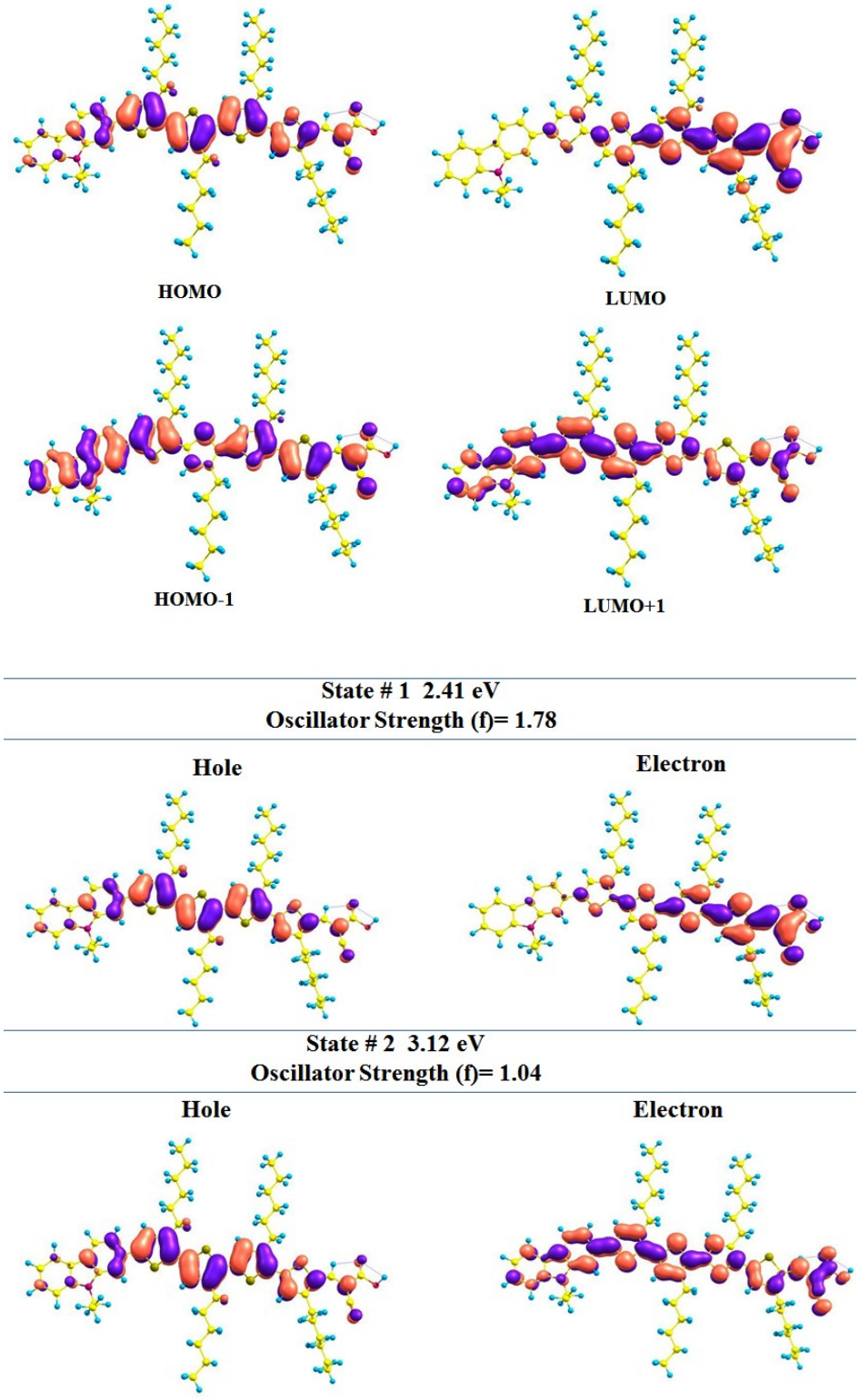


Figure S2. Simulated absorption spectra with oscillator strength (vertical lines) and experimental spectra of MK-2 in chloroform. Relevant molecular orbitals and natural transition orbitals (NTOs) for two lowest transitions of MK-2 dye.

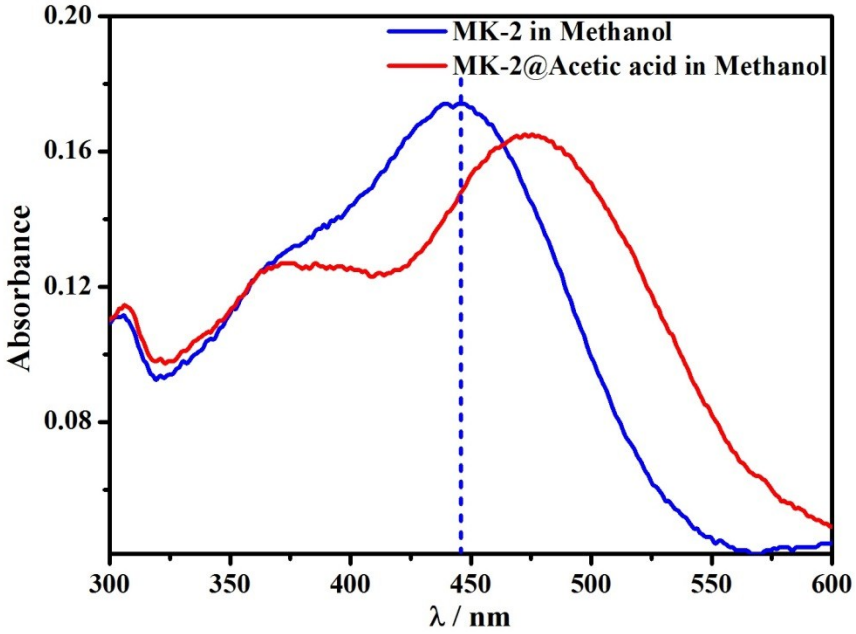


Figure S3. Absorption spectra of pure MK-2 dye and dye with acetic acid in methanol.

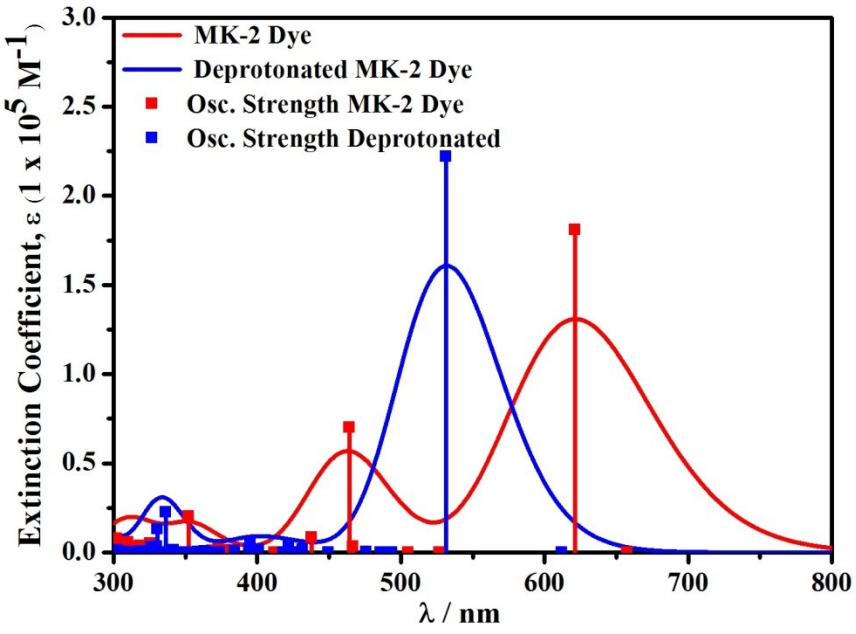


Figure S4. Simulated absorption spectra of nutral (red) and deprotonated MK-2 dye (blue) including oscillator strength in chloroform.

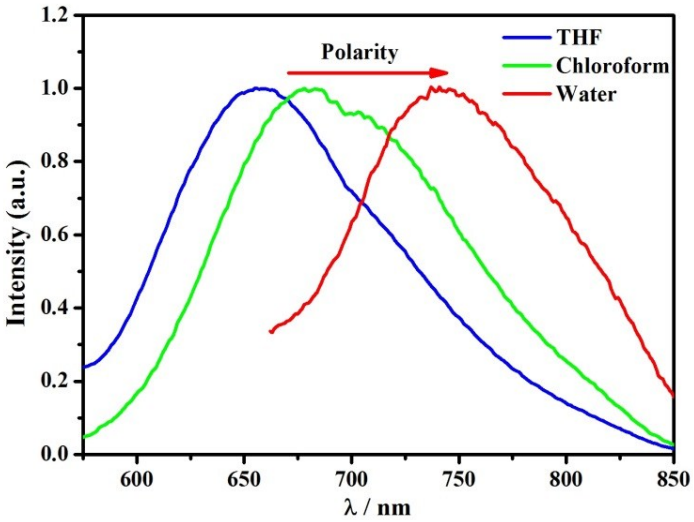
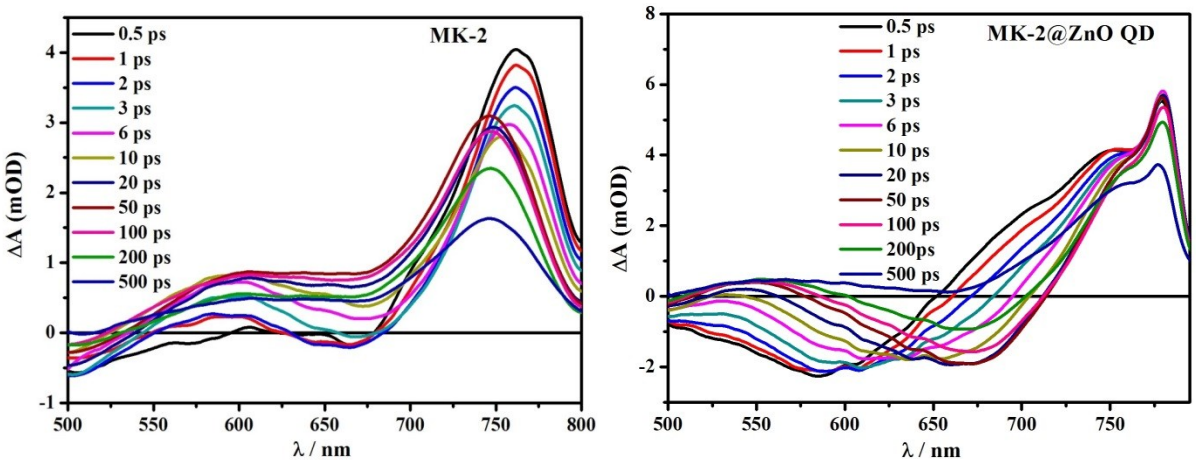


Figure S5. Emission spectra of MK-2 dye in different solvents.



(a) **(b)**

Figure S6. TA spectra of MK-2 dye and MK-2@ZnO QD measured at time delay from 0.5 ps to 500 ps.

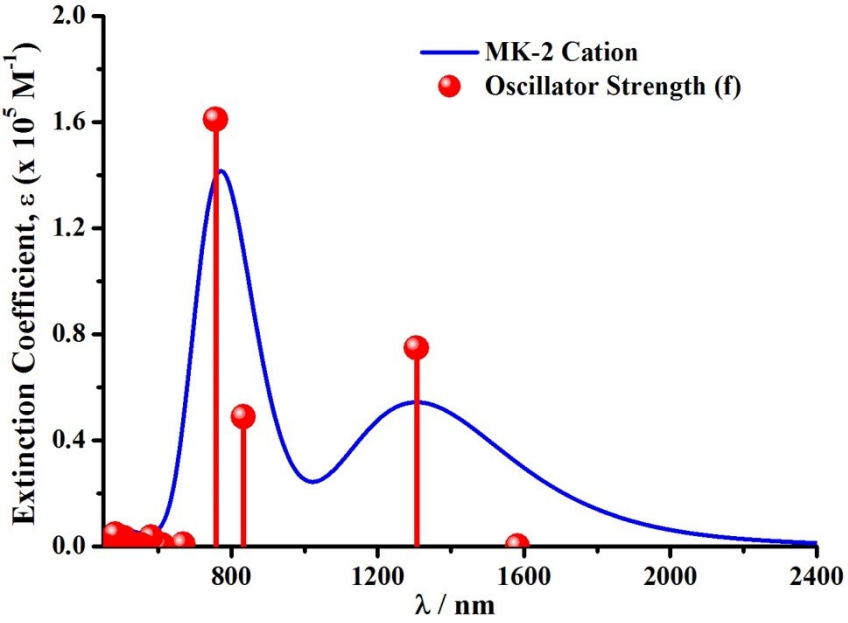


Figure S7. Simulated absorption spectra of the cation radical of MK-2 (MK-2 $^{\bullet+}$) with major vertical transitions obtained by TD-DFT/ B3LYP/ LanL2DZ/ IEFPCM in chloroform.

Figure S8. Molecular structures of dye anchored ZnO nanocluster before and after geometry optimization.