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

Nanoparticle and Surfactant Controlled Switching between Proton Transfer and Charge Transfer Reaction Coordinates

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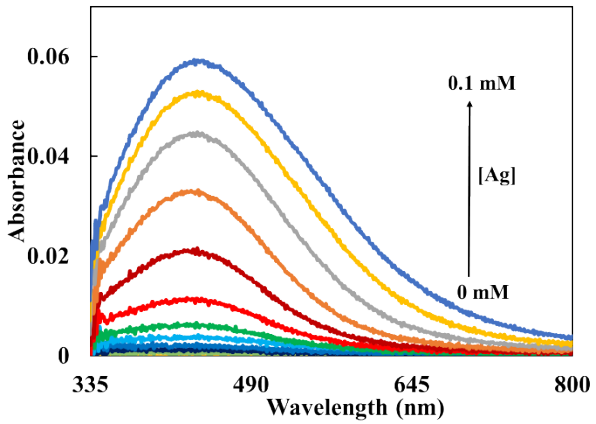


Figure S1. The SPR band of silver nanoparticle at different concentration (0 to 0.1 mM).

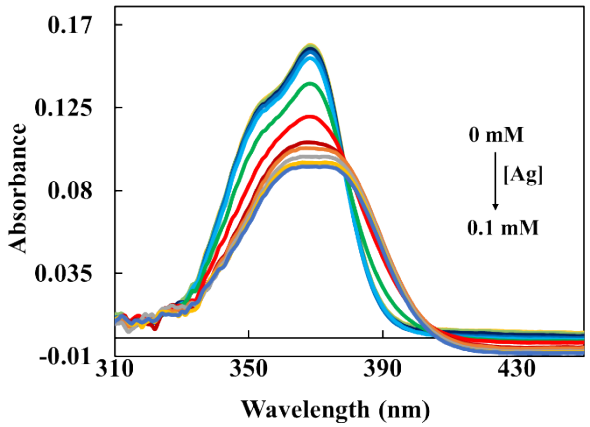


Figure S2. The absorption spectra of DHP in the presence of silver particle (0 to 0.1 mM) with silver particles reference.

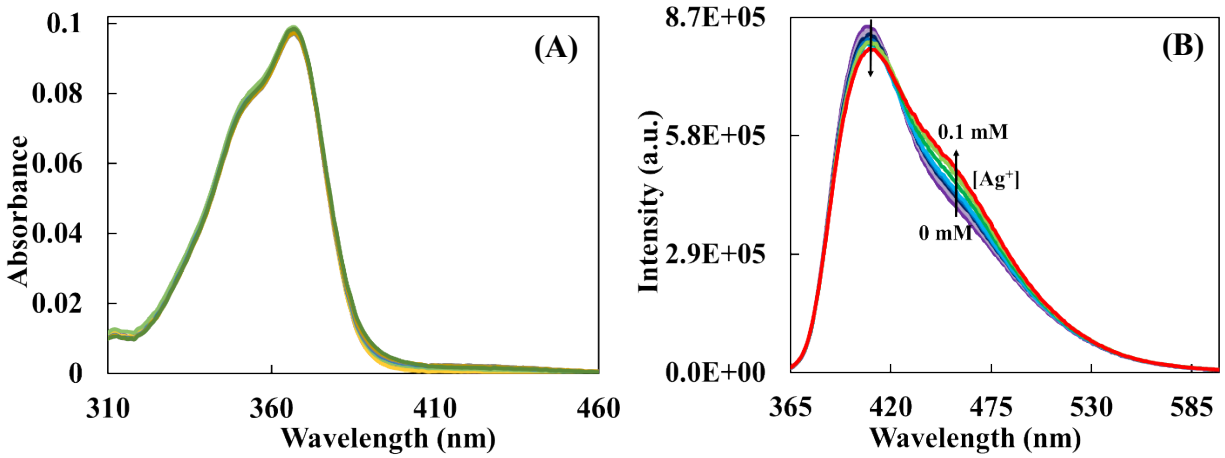


Figure S3. (A) Absorption spectra and **(B)** emission spectra of DHP in presence of different concentration of Ag^+ ion (0 to 0.1 mM) in acetonitrile, λ_{exc} = 350 nm.

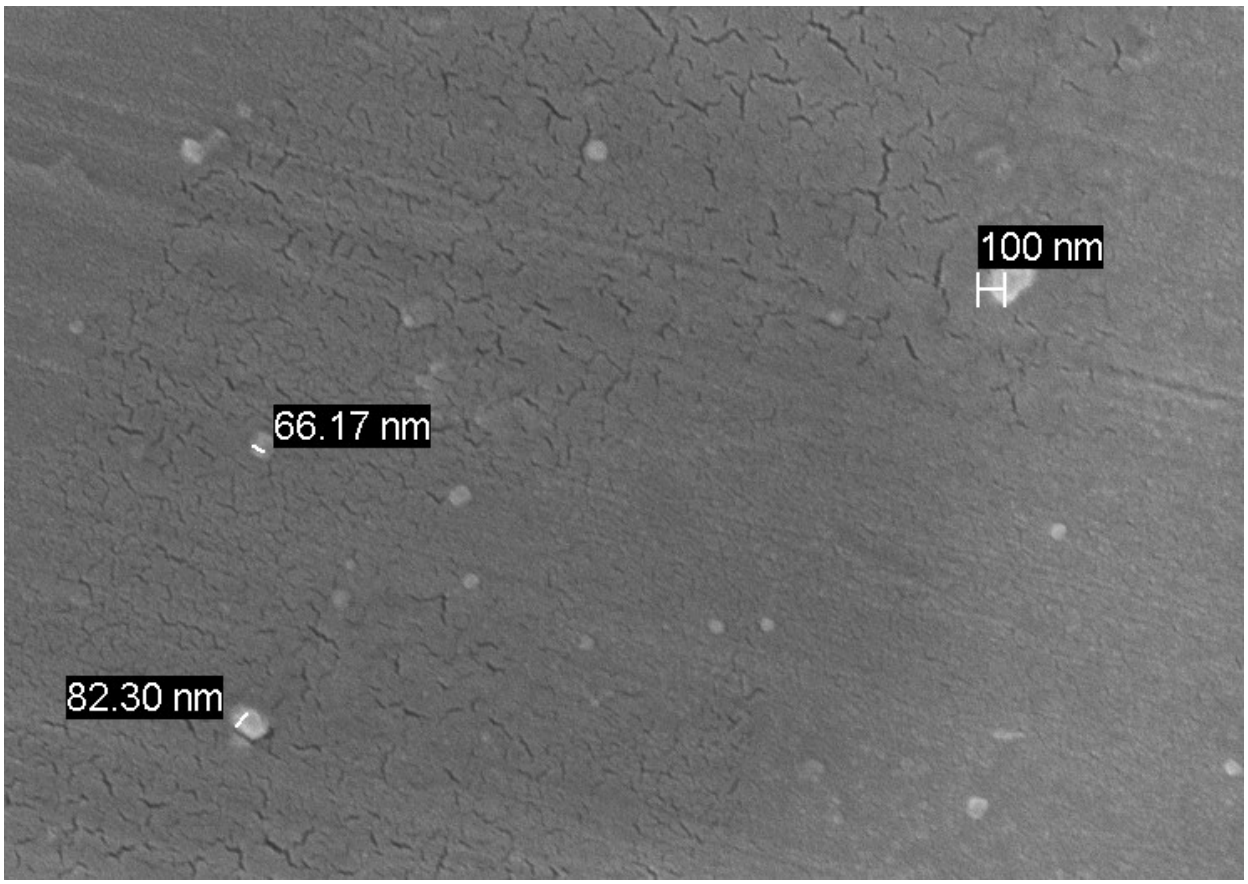
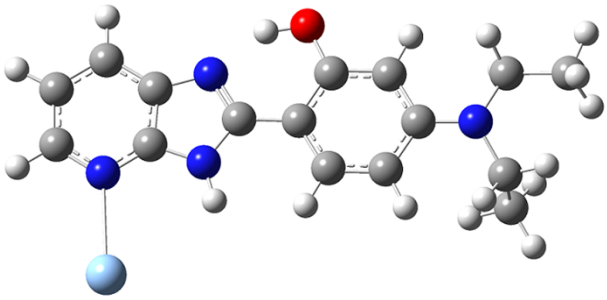


Figure S4. The FESEM image of silver nanoparticles in presence of DHP.

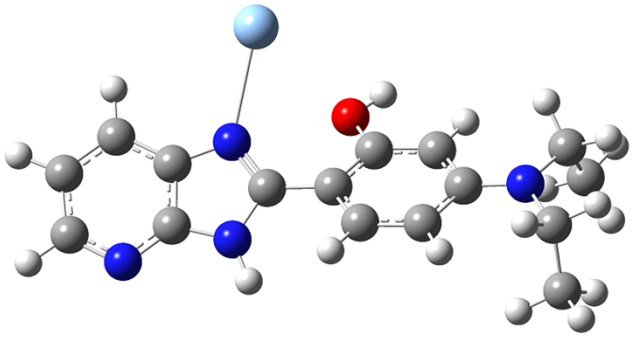
Table S1. Optimized geometries of DHP-silver complex and their Cartesian coordinates.



Energy (Hartree) : -1061.423113

N	3.79391567	0.51500724	0.07622115
C	4.70642336	1.50199867	0.16480058
C	4.37403419	2.86518589	0.22956191
C	3.03514742	3.27466449	0.20408187
C	2.07429574	2.26464196	0.11241038
C	2.52946993	0.92147861	0.05317264
N	1.39140784	0.14871758	-0.03228348
C	0.30731506	1.00093482	-0.02411099
N	0.69440672	2.28033757	0.06267156
C	-1.07580162	0.58656809	-0.09655811
C	-1.47192259	-0.76612033	-0.19045368
C	-2.79735010	-1.15017366	-0.24926294
C	-3.84422051	-0.17667962	-0.22861915
C	-3.45573568	1.18006413	-0.11594865
C	-2.11390039	1.56084439	-0.06051095
N	-5.17378027	-0.54134261	-0.32721910
C	-5.56060210	-1.93922102	-0.10888774
C	-5.57040209	-2.35005849	1.36489230
C	-6.19314391	0.50634985	-0.14587069
C	-7.63077318	0.07108472	-0.40217346
O	-1.84346703	2.88529921	0.03858406
Ag	4.33842243	-2.03459980	-0.09659599
H	5.75207822	1.18276358	0.18436614
H	5.17580669	3.60259117	0.29994428
H	2.75483241	4.32878048	0.25295828
H	1.37573744	-0.86433895	-0.08640935
H	-0.71391221	-1.55251641	-0.21600802
H	-3.02285069	-2.21186183	-0.31187707
H	-4.18452903	1.98503102	-0.06581006
H	-6.55151412	-2.09402523	-0.55133312
H	-4.89021646	-2.58899499	-0.68759828
H	-5.95915724	1.32351131	-0.84542659
H	-6.11549795	0.93523059	0.87267914
H	-6.28113397	-1.73513532	1.93952984

H	-5.86821162	-3.40528970	1.47054147
H	-4.57294034	-2.22736722	1.81481080
H	-7.75674774	-0.35176648	-1.41116366
H	-7.99355652	-0.66190003	0.33356262
H	-8.27896012	0.95747957	-0.32785304
H	-0.84599591	2.99319161	0.07155475



Energy (Hartree): -1061.412967

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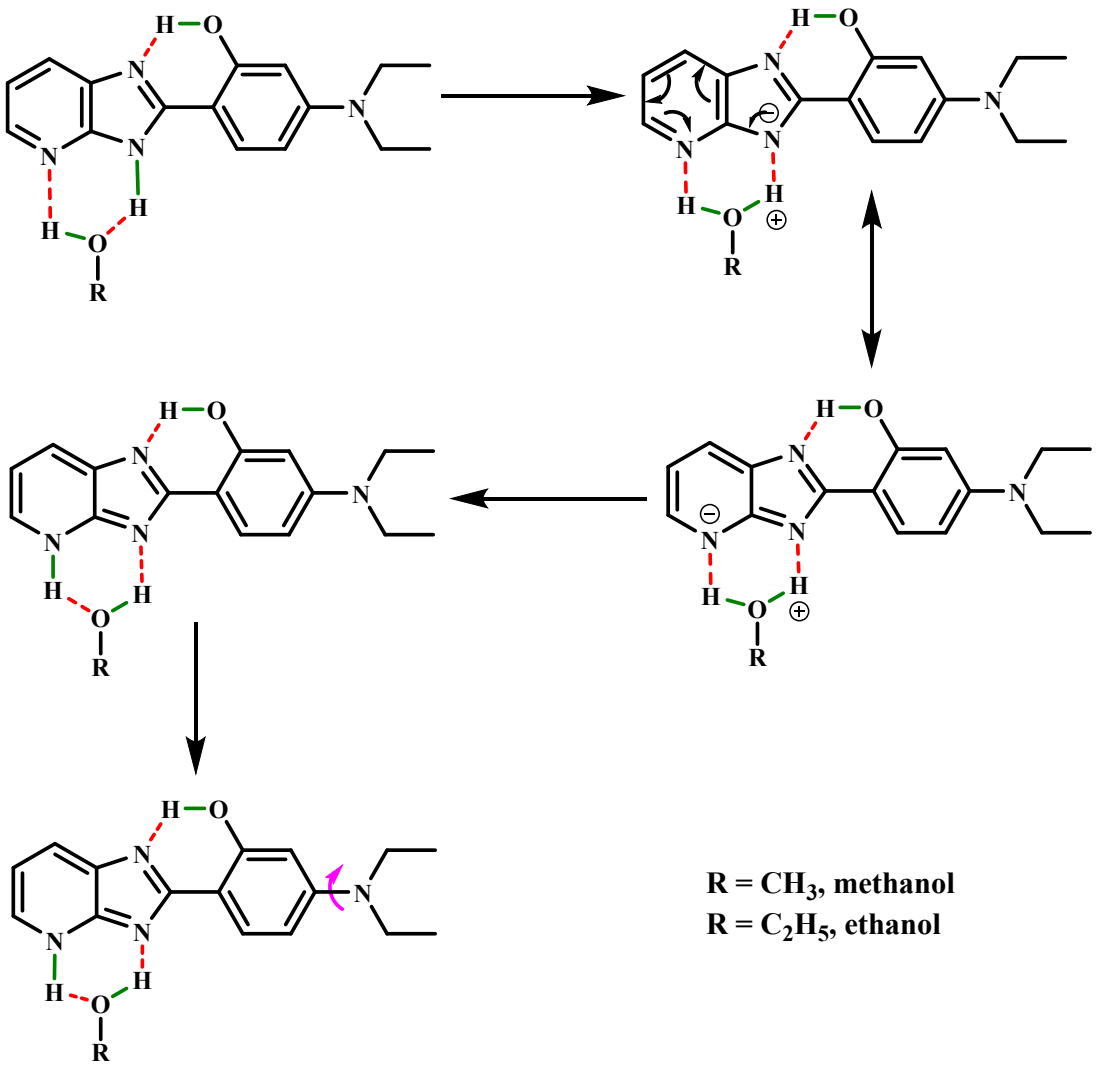
C	-5.51845752	1.30568751	0.31077446
C	-4.54902556	0.29784857	0.31139713
C	-3.21815043	0.71837270	0.24361055
C	-2.96433560	2.11230947	0.17019903
N	-1.59122449	2.21925391	0.10000620
C	-1.06312301	0.94102672	0.13245924
N	-2.02424801	0.02314603	0.21998408
C	0.37201359	0.70327226	0.02422495
C	1.19109075	1.59308257	-0.70496078
C	2.55581891	1.41553495	-0.85440518
C	3.21006700	0.29326578	-0.26899255
C	2.39810455	-0.59447874	0.48270655
C	1.02549669	-0.39966502	0.62709057
N	4.55688875	0.06917367	-0.43949766
C	5.40495334	1.05606948	-1.11408156
C	5.77323182	2.27242196	-0.25950835
C	5.22388186	-1.05779123	0.21645462
C	5.56077710	-0.83064938	1.69339880
O	0.28223486	-1.25392167	1.38979354
Ag	-1.89491951	-2.44290952	-0.47936271
H	-5.90793145	3.43993986	0.24827508
H	-6.57965175	1.05432831	0.36178188
H	-4.80832283	-0.76221763	0.35970543
H	-1.06477140	3.08623951	0.10352605
H	0.73129100	2.44912875	-1.20456262
H	3.11072329	2.14417628	-1.44074104
H	2.83449495	-1.45463819	0.98852718
H	6.31952737	0.53295280	-1.42872448
H	4.91169489	1.38024296	-2.04409706

H	6.14653022	-1.26074018	-0.34671055
H	4.60089569	-1.95894596	0.10147857
H	6.36058501	1.97619946	0.62215764
H	6.37554681	2.98185348	-0.84905804
H	4.87369062	2.79972433	0.09301651
H	6.27653018	-0.00421431	1.81471596
H	4.65989311	-0.58720505	2.27716740
H	6.01185297	-1.73882379	2.12388462
H	0.84960495	-1.96068385	1.73834505



Scheme S1. Intermolecular proton transfer triggered TICT emission in DHP.

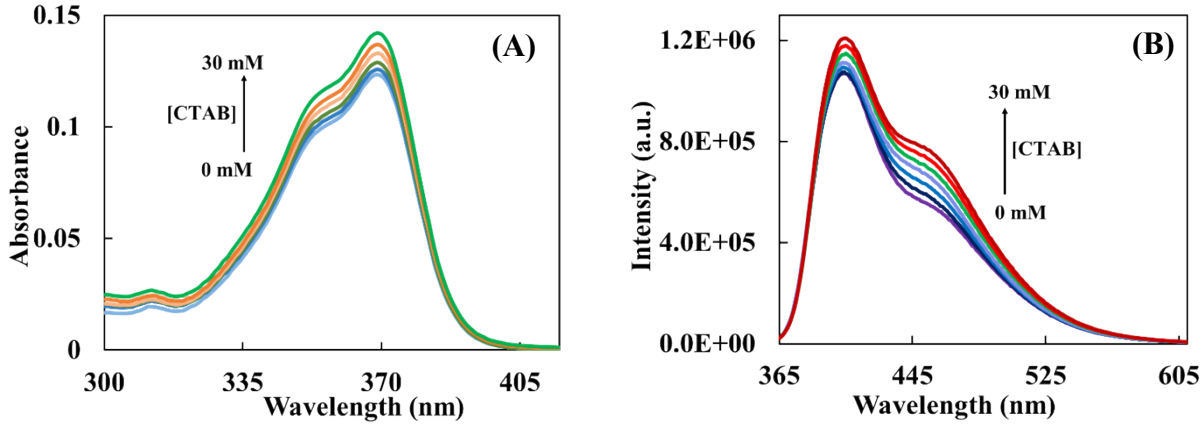


Figure S5. (A) Absorption spectra and **(B)** emission spectra of DHP in presence of different concentrations of CTAB (0 to 30 mM), λ_{exc} = 350 nm.

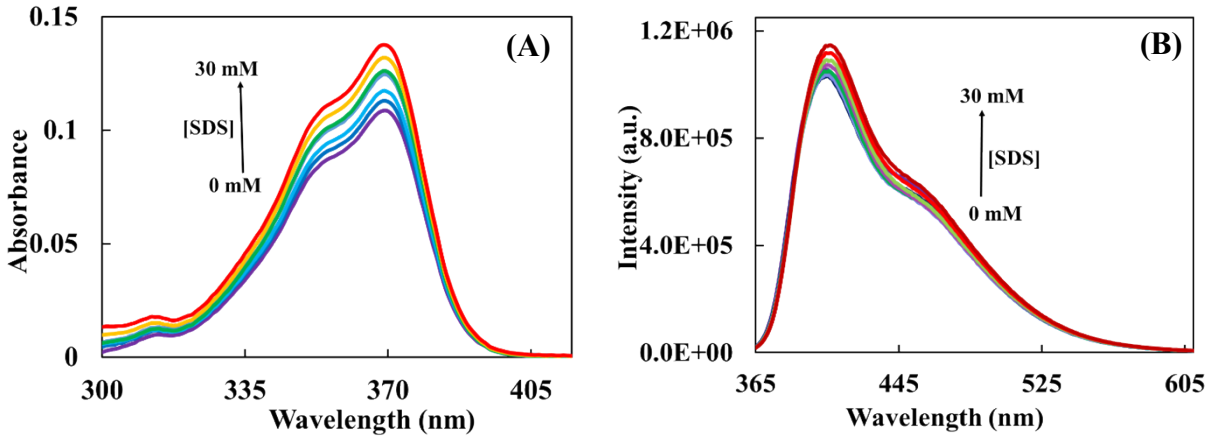


Figure S6. (A) Absorption spectra and **(B)** emission spectra of DHP in presence of different concentrations of SDS (0 to 30 mM), λ_{exc} = 350 nm.

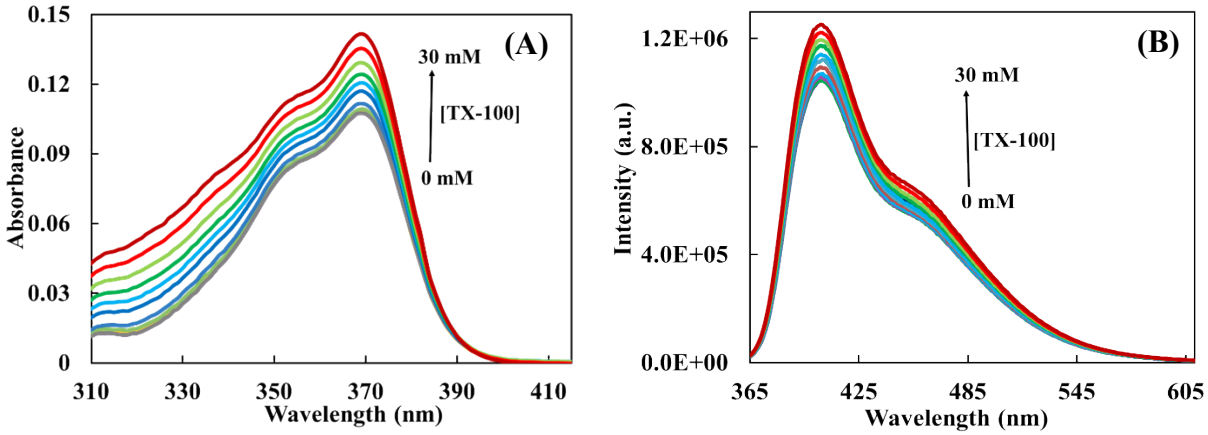


Figure S7. (A) Absorption spectra and **(B)** emission spectra of DHP in presence of different concentrations of TX-100 (0 to 30 mM), λ_{exc} = 350 nm.

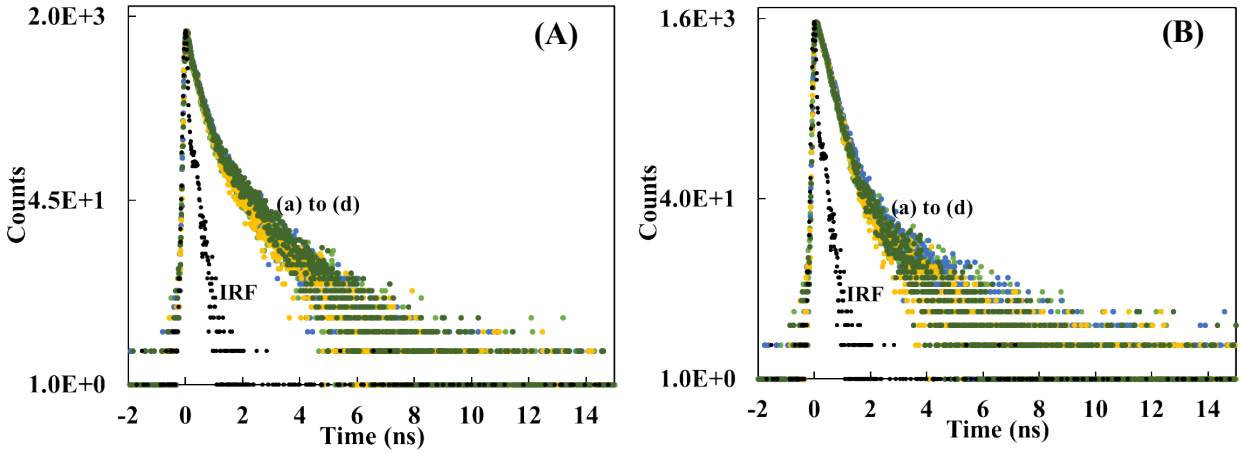


Figure S8. The fluorescence decays of DHP (a) in absence of surfactants, (b) in presence of 30 mM CTAB, (c) in presence of 30 mM SDS and (d) in presence of 30 mM TX-100 at **(A)** λ_{em} = 406 nm and **(B)** λ_{em} = 460 nm in DMF, λ_{exc} = 375 nm.

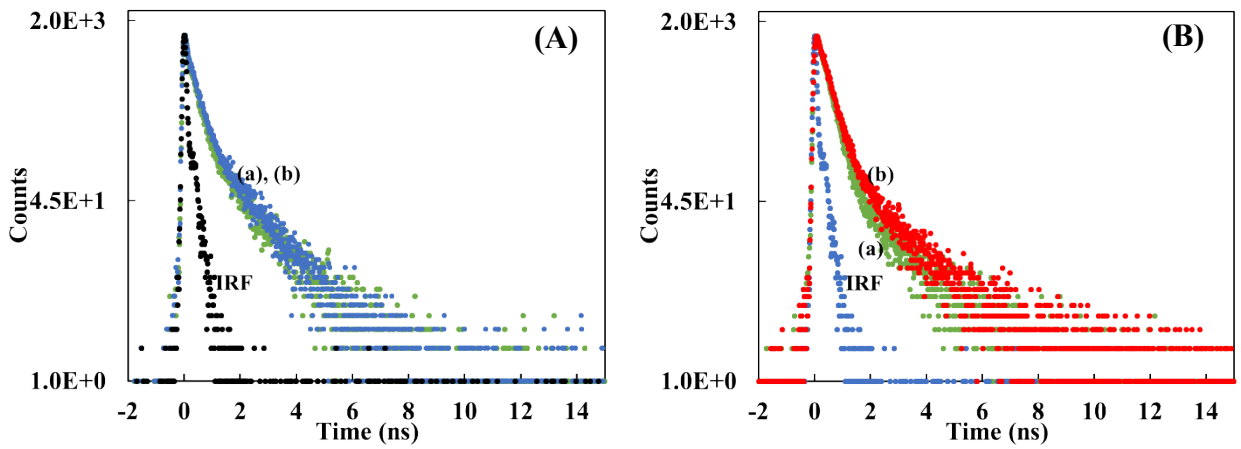


Figure S9: The fluorescence decays of DHP in (a) absence and (b) presence of 0.1 mM nanoparticle and 30 mM SDS at **(A)** λ_{em} = 406 nm and **(B)** λ_{em} = 460 nm in DMF, λ_{exc} = 375 nm.

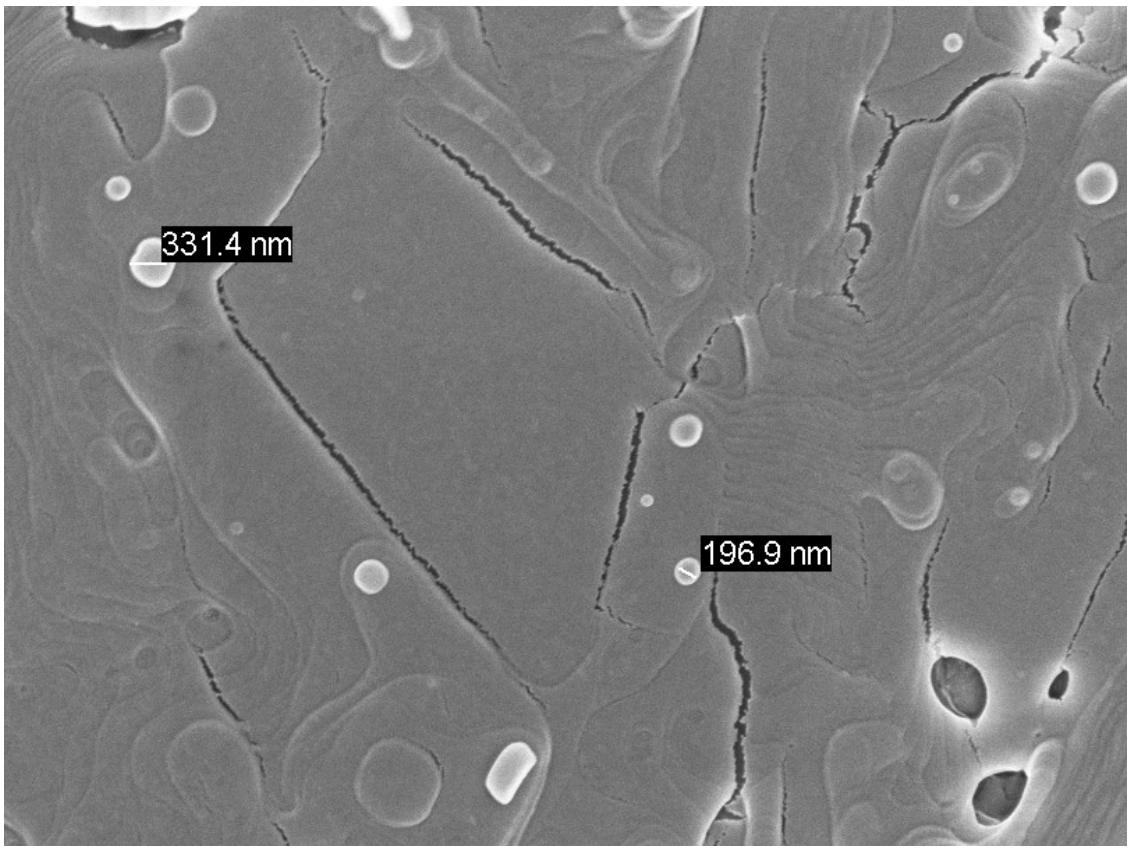


Figure S10. The FESEM images of silver nanoparticles in presence of both SDS and DHP.

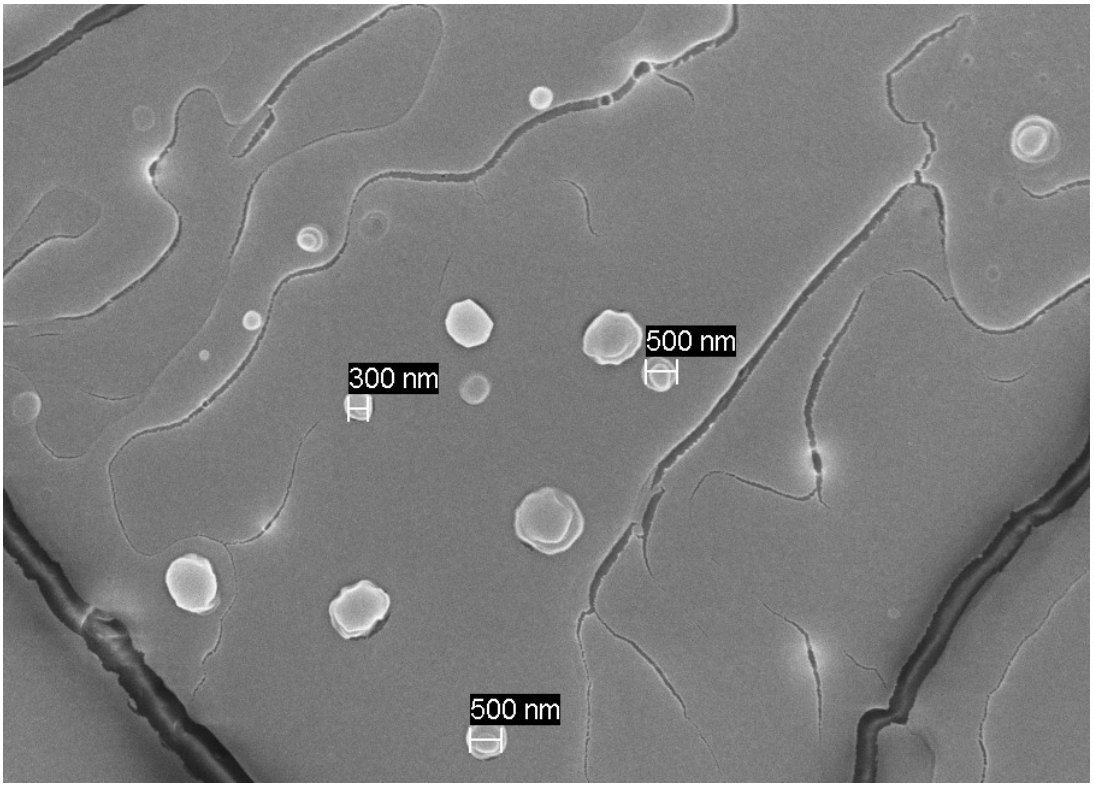


Figure S11. The FESEM images of silver nanoparticles in presence of SDS.

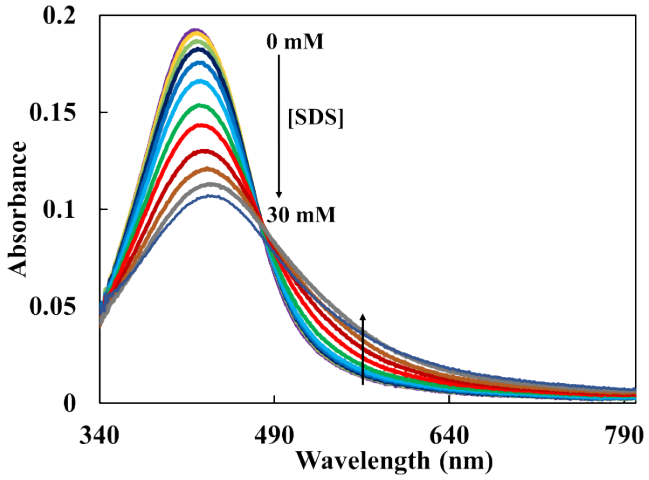


Figure S12. The absorption spectra of silver nanoparticle in presence of SDS (0 to 30 mM).

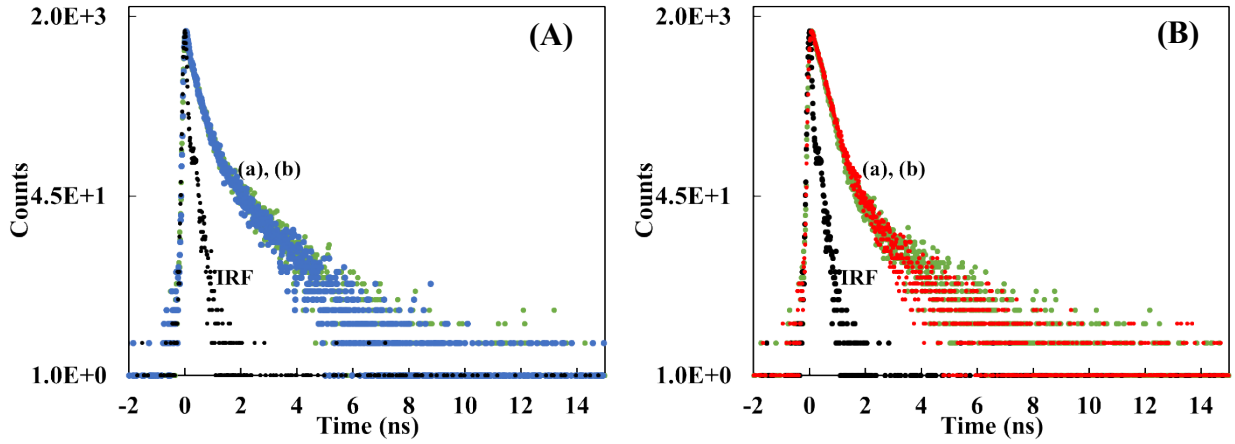


Figure S13. The fluorescence decays of DHP in (a) absence and (b) presence of 0.1 mM nanoparticle and 30 mM TX-100 at **(A)** λ_{em} = 406 nm and **(B)** λ_{em} = 460 nm in DMF, λ_{exc} = 375 nm.

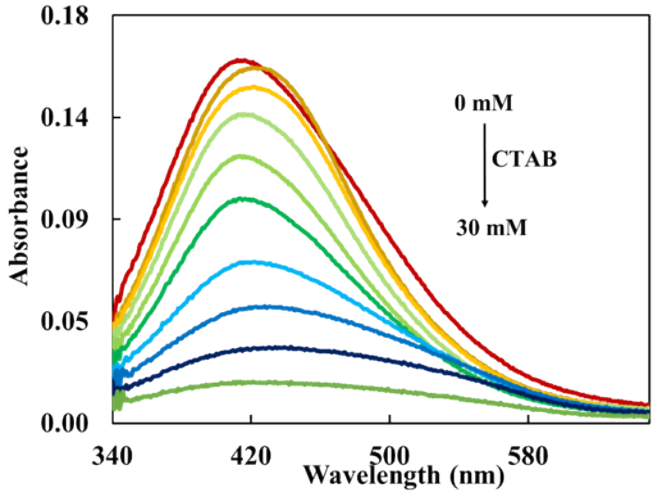


Figure S14. The absorption spectra of silver nanoparticle in presence of CTAB (0 to 30 mM).