Electronic Supplementary Information

The effect of heavy atoms on the deactivation of electronic excited states of dye molecules near the surface of metal nanoparticles

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The dianionic form of fluorescein, 2Br-fluorescein, eosin, and erythrosin dyes was chosen. Optimization of the molecular geometry in the S_1 were performed using the density functional theory (DFT) and time-dependent DFT (TD DFT) methods with the B3LYP/6-31++G(d,p) basis set and polarizable continuum model (PCM) with ethanol as solvent. The calculations were carried out with Gaussian 16.

The coordinates of the atoms in the studied dyes after structure optimization are presented below.

Fluorescein

C	3.699456000	0.339035000	0.180638000
C	2.342577000	0.538081000	0.023236000
O	1.928644000	1.851121000	-0.007895000
C	1.402889000	-0.533329000	-0.089497000
C	0.004410000	-0.257010000	-0.251422000
C	-0.386886000	1.126953000	-0.299855000
C	0.595251000	2.155308000	-0.174652000
C	4.258743000	-0.988069000	0.255364000
C	1.955855000	-1.850611000	0.022111000
C	-1.726222000	1.578790000	-0.526348000
C	0.290971000	3.501496000	-0.228995000
C	-1.062475000	3.955625000	-0.433868000
C	-2.059438000	2.912959000	-0.588484000
H	-2.502011000	0.832136000	-0.655412000
H	1.084008000	4.235817000	-0.126972000
C	3.303908000	-2.078383000	0.179384000
H	4.362616000	1.195085000	0.257460000
H	1.274581000	-2.693689000	-0.013413000
C	-0.973195000	-1.348366000	-0.455206000
C	-2.076563000	-1.587270000	0.406410000
C	-0.828369000	-2.165321000	-1.598693000
C	-2.990778000	-2.600701000	0.077281000
C	-1.731207000	-3.185293000	-1.895069000
C	-2.826211000	-3.405424000	-1.051427000
H	0.001479000	-1.974575000	-2.273959000
H	-3.837170000	-2.756690000	0.738835000
H	-1.589270000	-3.791698000	-2.785511000
H	-3.542652000	-4.192047000	-1.271397000
C	-2.286049000	-0.845709000	1.731522000
O	-1.255275000	-0.578549000	2.411517000
O	-3.484769000	-0.596973000	2.056349000
H	-3.088212000	3.218036000	-0.759636000
H	3.687144000	-3.091586000	0.264738000
O	5.510403000	-1.189998000	0.393486000
O	-1.360320000	5.194732000	-0.487120000

2Br-fluorescein

C	1.730357000	-2.240813000	0.045232000
C	0.818644000	-1.200993000	-0.072273000
O	1.331782000	0.070905000	-0.077409000
C	-0.582595000	-1.432797000	-0.170361000
C	-1.481212000	-0.322605000	-0.298191000
C	-0.908100000	0.993833000	-0.333829000
C	0.500556000	1.153791000	-0.214599000
C	1.318884000	-3.632592000	0.090026000

C	-1.004200000	-2.799298000	-0.091794000
C	-1.667074000	2.192437000	-0.523685000
C	1.105823000	2.403224000	-0.240680000
C	0.345450000	3.628741000	-0.411251000
C	-1.083466000	3.434146000	-0.558320000
H	-2.741178000	2.104897000	-0.640903000
C	-0.114800000	-3.838184000	0.024413000
H	-2.067672000	-3.007759000	-0.122917000
C	-2.937614000	-0.534817000	-0.465558000
C	-3.898091000	-0.074014000	0.469517000
C	-3.390776000	-1.189269000	-1.630540000
C	-5.261607000	-0.266779000	0.196471000
C	-4.748464000	-1.395808000	-1.874112000
C	-5.693453000	-0.930169000	-0.953514000
H	-2.658565000	-1.524703000	-2.360271000
H	-5.987449000	0.106000000	0.912845000
H	-5.064919000	-1.903483000	-2.781056000
H	-6.754852000	-1.079373000	-1.131238000
C	-3.521557000	0.573480000	1.806170000
O	-4.178921000	1.602859000	2.136859000
O	-2.618869000	0.005970000	2.484184000
O	2.138074000	-4.592401000	0.189653000
O	0.879051000	4.776331000	-0.439234000
Br	3.581784000	-1.862125000	0.163822000
Br	2.985541000	2.542250000	-0.060074000
H	-0.465039000	-4.864511000	0.083944000
H	-1.685829000	4.326161000	-0.702765000

Erythrosin

C	-2.475195000	-1.381023000	-0.061168000
C	-1.283597000	-0.675242000	-0.084606000
O	-0.117945000	-1.399789000	-0.035055000
C	-1.252993000	0.749724000	-0.148471000
C	0.000797000	1.439007000	-0.185041000
C	1.194587000	0.645326000	-0.162044000
C	1.104800000	-0.775223000	-0.077320000
C	-3.780077000	-0.729258000	-0.089282000
C	-2.513704000	1.418057000	-0.134780000
C	2.505256000	1.199544000	-0.254054000
C	2.232606000	-1.579550000	-0.045010000
C	3.587457000	-1.042442000	-0.114022000
C	3.629180000	0.409427000	-0.232810000
H	2.598769000	2.274103000	-0.347948000
C	-3.699848000	0.725400000	-0.111874000
H	-2.515052000	2.500649000	-0.139550000
C	0.058592000	2.915447000	-0.315958000
C	0.575785000	3.758507000	0.698238000
C	-0.383430000	3.497716000	-1.521814000
C	0.644215000	5.141167000	0.463598000
C	-0.332812000	4.876870000	-1.728812000
C	0.185175000	5.705960000	-0.728047000
H	-0.760124000	2.850220000	-2.309415000
H	1.058853000	5.773616000	1.242581000
H	-0.683772000	5.297063000	-2.667310000
H	0.234778000	6.781227000	-0.876492000
C	1.017996000	3.234544000	2.069199000
O	0.307536000	2.331444000	2.594663000

O	2.044017000	3.776590000	2.574457000
O	-4.865042000	-1.365166000	-0.085302000
O	4.615261000	-1.766425000	-0.082306000
I	-5.540259000	1.798575000	-0.098775000
I	-2.474544000	-3.496011000	0.020178000
I	2.052134000	-3.683139000	0.111752000
I	5.549597000	1.318426000	-0.373702000

Eosin

C	1.756375000	-0.032232000	2.348813000
C	1.002388000	-0.072253000	1.189821000
O	1.680769000	-0.001729000	0.000000000
C	-0.417993000	-0.173780000	1.222620000
C	-1.155199000	-0.202624000	0.000000000
C	-0.417993000	-0.173780000	-1.222620000
C	1.002388000	-0.072253000	-1.189821000
C	1.166895000	-0.094568000	3.678508000
C	-1.030292000	-0.231672000	2.507369000
C	-1.030292000	-0.231672000	-2.507369000
C	1.756375000	-0.032232000	-2.348813000
C	1.166895000	-0.094568000	-3.678508000
C	-0.284090000	-0.194032000	-3.660969000
H	-2.109932000	-0.301578000	-2.562688000
C	-0.284090000	-0.194032000	3.660969000
H	-2.109932000	-0.301578000	2.562688000
C	-2.629979000	-0.407392000	0.000000000
C	-3.576076000	0.643847000	0.000000000
C	-3.087984000	-1.739214000	0.000000000
C	-4.942357000	0.318094000	0.000000000
C	-4.450101000	-2.043431000	0.000000000
C	-5.385013000	-1.004628000	0.000000000
H	-2.356584000	-2.543193000	0.000000000
H	-5.650709000	1.139102000	0.000000000
H	-4.774587000	-3.080239000	0.000000000
H	-6.449277000	-1.223481000	0.000000000
C	-3.182384000	2.131072000	0.000000000
O	-1.950015000	2.406697000	0.000000000
O	-4.134526000	2.965117000	0.000000000
O	1.852707000	-0.065204000	4.733499000
O	1.852707000	-0.065204000	-4.733499000
Br	-1.166082000	-0.279075000	5.343140000
Br	3.639983000	0.104812000	2.245420000
Br	3.639983000	0.104812000	-2.245420000
Br	-1.166082000	-0.279075000	-5.343140000