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New di-anchoring A- π -D- π -A configured organic chromophores for DSSC application: Sensitization and co-sensitization studies

Praveen Naik^a, Rui Su^b, Mohamed R. Elmorsy^b, Ahmed El-Shafei^{b,*} Airody Vasudeva Adhikari^{a,*} ^aOrganic Materials Laboratory, Department of Chemistry, National Institute of Technology Karnataka, Surathkal, Mangalore-575 025, India

(Corresponding Author: A. Vasudeva Adhikari, <u>avachem@gmail.com</u>) ^bPolymer and Color Chemistry Program, North Carolina State University, Raleigh, NC, 27695, USA (Corresponding Author: Ahmed El-Shafei, <u>ahmed_el-shafei@ncsu.edu</u>)

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1. DFT calculations

| 1 2 |
|-----|
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| ATOM | CARTESI | AN GRADIENTS | |
|------|-------------------|-------------------|-------------------|
| 1 c | 0.00003784479301 | -0.00001721620721 | 0.00008037745832 |
| 2 c | -0.00002016945915 | 0.00001900189193 | 0.00006431442518 |
| 3 c | 0.00000846942457 | -0.00001388535052 | -0.00000720712743 |
| 4 c | 0.00000433419569 | -0.00003129992040 | -0.00013413496263 |
| 5 c | -0.00002110354363 | -0.00001933469122 | -0.00009033763747 |
| 6 c | -0.00001826282021 | -0.00001180783970 | -0.00000706393747 |
| 7 n | 0.00004556216265 | -0.00000908626126 | 0.00006061610172 |
| 8 c | -0.00001681132518 | 0.00001788402626 | -0.00003206539369 |
| 9 c | -0.00001926879675 | 0.00001087752220 | 0.00011747063877 |
| 10 c | -0.00000408884940 | 0.00001226139297 | -0.00002870284998 |
| 11 c | -0.00001788958345 | -0.00000636175783 | 0.00001673138529 |
| 12 c | 0.00000378766631 | -0.00000210567824 | 0.00000572506943 |
| 13 c | -0.00001367378643 | -0.00000132196599 | -0.00007853695908 |
| 14 c | -0.00000009222507 | -0.00001124065437 | 0.00003188350677 |
| 15 c | -0.00000018702574 | 0.00000240617247 | 0.00000158273095 |
| 16 c | -0.00001004742700 | 0.00000361630255 | -0.00000193160842 |
| 17 c | 0.00000250381739 | -0.00000390800281 | 0.00000447929225 |
| 18 c | -0.00000522481087 | 0.00000407200881 | -0.00000256976734 |
| 19 c | 0.00000483767251 | -0.00000182596659 | -0.00000170478502 |
| 20 c | -0.00005217216670 | 0.00003708232995 | 0.00003001931371 |
| 21 c | -0.00001455742162 | -0.00001244255667 | 0.00000125137517 |
| 22 c | 0.00000397043845 | 0.00001232810613 | 0.00000313973702 |
| 23 c | -0.00000573647627 | -0.00001164389911 | 0.00000364546866 |
| 24 c | 0.00001633102364 | -0.00001167119067 | 0.00001353220678 |
| 25 c | -0.00003410141801 | -0.00000976771990 | -0.00002658570803 |
| 26 c | 0.00001562924094 | -0.00001296888583 | 0.00000228946880 |
| 27 c | -0.00007022397351 | -0.00003277262123 | -0.00007828555223 |
| 28 c | 0.00003333028883 | 0.00001715112606 | -0.00000759197477 |

| 29 c | -0.00000588305224 | 0.00003330318697 | 0.00002960852630 | |
|------|-------------------|-------------------|-------------------|--|
| 30 c | 0.00003159515757 | -0.00007545815123 | 0.00003110847079 | |
| 31 n | -0.00002036528631 | 0.00003200809973 | 0.00003100825605 | |
| 32 c | 0.00002778031417 | -0.00001184455572 | -0.00007228208753 | |
| 33 o | -0.00000650941741 | 0.00002611569975 | -0.00003114799150 | |
| 34 o | -0.00001558121819 | 0.00001213065719 | 0.00004415291402 | |
| 35 c | 0.00001793681608 | 0.00001972908549 | -0.00001747608933 | |
| 36 n | -0.00000202035085 | -0.00001606343961 | 0.00000994454227 | |
| 37 c | 0.00002156307140 | 0.00001506379264 | 0.00007979387298 | |
| 38 o | -0.00004144893969 | 0.00007244930872 | -0.00005274083076 | |
| 39 o | 0.00002760514091 | -0.00003821491474 | 0.00002498291573 | |
| 40 h | 0.00000742091540 | -0.00002337891920 | -0.00008736524662 | |
| 41 h | 0.00000012335878 | 0.00000019413773 | 0.00005350850748 | |
| 42 h | 0.00000071521864 | -0.00000288427643 | -0.00004069994330 | |
| 43 h | 0.00000842353000 | -0.00000424644719 | -0.00003420305370 | |
| 44 h | 0.00000012624743 | -0.00001403468966 | 0.00001853798557 | |
| 45 h | -0.00000386181884 | 0.00002004927138 | 0.00011809479060 | |
| 46 h | 0.00001243431225 | 0.00000460341403 | 0.00000681760911 | |
| 47 h | -0.00000316876467 | -0.00000331101519 | 0.00000194490477 | |
| 48 h | 0.00001324372319 | -0.00001085815000 | -0.00000392693130 | |
| 49 h | -0.00000435810776 | -0.00000028702346 | -0.00000308148364 | |
| 50 h | 0.00000298483014 | 0.00000709955496 | -0.00000538613454 | |
| 51 h | -0.00000588143288 | 0.00000176066108 | 0.00000571482880 | |
| 52 h | 0.00000704658212 | -0.00000513786615 | -0.00000037433829 | |
| 53 h | -0.00000466780828 | -0.00000675967949 | -0.00000078322364 | |
| 54 h | -0.00000515530342 | 0.00000454075195 | -0.00000438756596 | |
| 55 h | -0.00000168114768 | 0.00000633408724 | 0.00000645023975 | |
| 56 h | -0.00000206815998 | 0.00000312289662 | 0.00000321666423 | |
| 57 h | 0.00000459215775 | -0.00000176467903 | 0.00000509695967 | |
| 58 h | -0.00000097849531 | -0.00000631348903 | -0.00000179567919 | |
| 59 h | -0.00000385090499 | -0.00004199627205 | -0.00006207685687 | |

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| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ |
| 65 h0.00001667531802-0.000031427992390.0000243565428966 h0.000042638309540.00000531522276-0.000018801867202.2Cartesian coordinates of the E2 dyeATOMCARTESIAN COORDINATES1 c-0.96475175506189-2.478783444308470.200642369846332 c1.68580827029287-2.37475055640676-0.049547590237663 c2.98796507279333-0.11322203480594-0.262238637838844 c1.596792786017352.11924859690638-0.225290607387845 c-1.061958592589692.077891332394190.023220875996076 c-2.32409249566061-0.214851474656440.236802510277697 n2.410673116997694.60999619084968-0.391861861744528 c0.330622519024196.17159022953244-0.284442591133369 c-1.885057594493754.68610543624312-0.0147881332190010 c0.186889795686508.80319723715156-0.3934087722958411 c-2.173707824232499.89692943234670-0.2143840515738912 c-4.425826731944558.465758860810270.07377846640855 |
| 66 h 0.00004263830954 0.00000531522276 -0.00001880186720 2.2 Cartesian coordinates of the E2 dye ATOM CARTESIAN COORDINATES 1 c -0.96475175506189 -2.47878344430847 0.20064236984633 2 c 1.68580827029287 -2.37475055640676 -0.04954759023766 3 c 2.98796507279333 -0.11322203480594 -0.26223863783884 4 c 1.59679278601735 2.11924859690638 -0.22529060738784 5 c -1.06195859258969 2.07789133239419 0.02322087599607 6 c -2.32409249566061 -0.21485147465644 0.23680251027769 7 n 2.41067311699769 4.60999619084968 -0.39186186174452 8 c 0.33062251902419 6.17159022953244 -0.28444259113336 9 c -1.88505759449375 4.68610543624312 -0.01478813321900 10 c 0.18688979568650 8.80319723715156 -0.39340877229584 11 c -2.17370782423249 9.89692943234670 -0.21438405157389 12 c -4.42582673194455 8.46575886081027 0.07377846640855 |
| 2.2Cartesian coordinates of the E_2 dyeATOMCARTESIAN COORDINATES1 c-0.96475175506189-2.478783444308470.200642369846332 c1.68580827029287-2.37475055640676-0.049547590237663 c2.98796507279333-0.11322203480594-0.262238637838844 c1.596792786017352.11924859690638-0.225290607387845 c-1.061958592589692.077891332394190.023220875996076 c-2.32409249566061-0.214851474656440.236802510277697 n2.410673116997694.60999619084968-0.391861861744528 c0.330622519024196.17159022953244-0.284442591133369 c-1.885057594493754.68610543624312-0.0147881332190010 c0.186889795686508.80319723715156-0.3934087722958411 c-2.173707824232499.89692943234670-0.2143840515738912 c-4.425826731944558.465758860810270.07377846640855 |
| ATOMCARTESIAN COORDINATES1 c-0.96475175506189-2.478783444308470.200642369846332 c1.68580827029287-2.37475055640676-0.049547590237663 c2.98796507279333-0.11322203480594-0.262238637838844 c1.596792786017352.11924859690638-0.225290607387845 c-1.061958592589692.077891332394190.023220875996076 c-2.32409249566061-0.214851474656440.236802510277697 n2.410673116997694.60999619084968-0.391861861744528 c0.330622519024196.17159022953244-0.284442591133369 c-1.885057594493754.68610543624312-0.0147881332190010 c0.186889795686508.80319723715156-0.3934087722958411 c-2.173707824232499.89692943234670-0.2143840515738912 c-4.425826731944558.465758860810270.07377846640855 |
| 1 c-0.96475175506189-2.478783444308470.200642369846332 c1.68580827029287-2.37475055640676-0.049547590237663 c2.98796507279333-0.11322203480594-0.262238637838844 c1.596792786017352.11924859690638-0.225290607387845 c-1.061958592589692.077891332394190.023220875996076 c-2.32409249566061-0.214851474656440.236802510277697 n2.410673116997694.60999619084968-0.391861861744528 c0.330622519024196.17159022953244-0.284442591133369 c-1.885057594493754.68610543624312-0.0147881332190010 c0.186889795686508.80319723715156-0.3934087722958411 c-2.173707824232499.89692943234670-0.2143840515738912 c-4.425826731944558.465758860810270.07377846640855 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ |
| 3 c2.98796507279333-0.11322203480594-0.262238637838844 c1.596792786017352.11924859690638-0.225290607387845 c-1.061958592589692.077891332394190.023220875996076 c-2.32409249566061-0.214851474656440.236802510277697 n2.410673116997694.60999619084968-0.391861861744528 c0.330622519024196.17159022953244-0.284442591133369 c-1.885057594493754.68610543624312-0.0147881332190010 c0.186889795686508.80319723715156-0.3934087722958411 c-2.173707824232499.89692943234670-0.2143840515738912 c-4.425826731944558.465758860810270.07377846640855 |
| 4 c1.596792786017352.11924859690638-0.225290607387845 c-1.061958592589692.077891332394190.023220875996076 c-2.32409249566061-0.214851474656440.236802510277697 n2.410673116997694.60999619084968-0.391861861744528 c0.330622519024196.17159022953244-0.284442591133369 c-1.885057594493754.68610543624312-0.0147881332190010 c0.186889795686508.80319723715156-0.3934087722958411 c-2.173707824232499.89692943234670-0.2143840515738912 c-4.425826731944558.465758860810270.07377846640855 |
| 5 c -1.06195859258969 2.07789133239419 0.02322087599607 6 c -2.32409249566061 -0.21485147465644 0.23680251027769 7 n 2.41067311699769 4.60999619084968 -0.39186186174452 8 c 0.33062251902419 6.17159022953244 -0.28444259113336 9 c -1.88505759449375 4.68610543624312 -0.01478813321900 10 c 0.18688979568650 8.80319723715156 -0.39340877229584 11 c -2.17370782423249 9.89692943234670 -0.21438405157389 12 c -4.42582673194455 8.46575886081027 0.07377846640855 |
| 6 c-2.32409249566061-0.214851474656440.236802510277697 n2.410673116997694.60999619084968-0.391861861744528 c0.330622519024196.17159022953244-0.284442591133369 c-1.885057594493754.68610543624312-0.0147881332190010 c0.186889795686508.80319723715156-0.3934087722958411 c-2.173707824232499.89692943234670-0.2143840515738912 c-4.425826731944558.465758860810270.07377846640855 |
| 7 n2.410673116997694.60999619084968-0.391861861744528 c0.330622519024196.17159022953244-0.284442591133369 c-1.885057594493754.68610543624312-0.0147881332190010 c0.186889795686508.80319723715156-0.3934087722958411 c-2.173707824232499.89692943234670-0.2143840515738912 c-4.425826731944558.465758860810270.07377846640855 |
| 8 c 0.33062251902419 6.17159022953244 -0.28444259113336 9 c -1.88505759449375 4.68610543624312 -0.01478813321900 10 c 0.18688979568650 8.80319723715156 -0.39340877229584 11 c -2.17370782423249 9.89692943234670 -0.21438405157389 12 c -4.42582673194455 8.46575886081027 0.07377846640855 |
| 9 c -1.88505759449375 4.68610543624312 -0.01478813321900 10 c 0.18688979568650 8.80319723715156 -0.39340877229584 11 c -2.17370782423249 9.89692943234670 -0.21438405157389 12 c -4.42582673194455 8.46575886081027 0.07377846640855 |
| 10 c0.186889795686508.80319723715156-0.3934087722958411 c-2.173707824232499.89692943234670-0.2143840515738912 c-4.425826731944558.465758860810270.07377846640855 |
| 11 c-2.173707824232499.89692943234670-0.2143840515738912 c-4.425826731944558.465758860810270.07377846640855 |
| 12 c -4.42582673194455 8.46575886081027 0.07377846640855 |
| |
| 13 c -4.23704572359043 5.81935110533922 0.16868636497748 |
| 14 c 5.00808747810742 5.42009585430454 -0.75822679515189 |
| 15 c 5.78224010130718 5.62425154167306 -3.53960724973537 |
| 16 c 8.52223812620967 6.47978576386703 -3.85904286740343 |
| 17 c 9.33674373959207 6.71880416119976 -6.62206847264974 |
| 18 c 12.07817858352985 7.57255989155938 -6.94591611629296 |
| 19 c 12.87815886619528 7.81628042656427 -9.70935259391795 |
| 20 c -6.74217831679539 9.91800512151998 0.23449404313327 |

| 21 c | -2.27249961489022 | -4.93569882655144 | 0.42466332007583 | |
|------|--------------------|--------------------|-------------------|--|
| 22 c | -4.46411216350196 | -5.19645525406427 | 1.88995835890302 | |
| 23 c | -5.67768653389895 | -7.49741808958404 | 2.09129874717865 | |
| 24 c | -4.77569616342393 | -9.67418055569169 | 0.85138839667220 | |
| 25 c | -2.57906322000127 | -9.41065163741219 | -0.62125687911282 | |
| 26 c | -1.37724012129474 | -7.09864412690214 | -0.81835158076143 | |
| 27 c | -6.23377014884142 | -11.96627213285419 | 1.23276345508029 | |
| 28 c | -9.22931685444362 | 9.38434501837643 | 0.55693438549560 | |
| 29 s | -11.45139058431339 | 11.93567502219384 | 0.62509176588228 | |
| 30 c | -14.07011650068798 | 9.85029555312959 | 1.11028007688428 | |
| 31 n | -13.15033746602968 | 7.41122438613992 | 1.18964733557415 | |
| 32 c | -10.57761662850366 | 6.96099865723670 | 0.90676614978610 | |
| 33 o | -16.24342368925338 | 10.46618572495800 | 1.32685032808826 | |
| 34 o | -9.71695777463510 | 4.83240538613116 | 0.96737294982821 | |
| 35 c | -6.05323630370863 | -14.40469061414079 | 0.47484325826874 | |
| 36 c | -4.16211675668726 | -15.71628967708825 | -1.12368225342319 | |
| 37 n | -4.79492585853616 | -18.25617954671453 | -1.33625111756161 | |
| 38 c | -6.92521245866104 | -19.17881398840711 | -0.14858147297815 | |
| 39 s | -8.40706858871736 | -16.61044313758445 | 1.48346750487829 | |
| 40 o | -2.30445127098531 | -14.84651223112572 | -2.14828367322197 | |
| 41 o | -7.65951771974819 | -21.32432930827517 | -0.19833982002800 | |
| 42 h | 2.75202381540310 | -4.11752698075908 | -0.02941647937770 | |
| 43 h | 5.02394177525743 | -0.11375242881909 | -0.43808253229300 | |
| 44 h | -4.36323291232204 | -0.24223316141733 | 0.37917154648799 | |
| 45 h | 1.85098634451724 | 9.96664327318521 | -0.61689767255358 | |
| 46 h | -2.31787906930428 | 11.93633143112143 | -0.29785873137917 | |
| 47 h | -5.92523381626567 | 4.70100691635792 | 0.38871066448488 | |
| 48 h | 5.24594549137193 | 7.23884262166391 | 0.18555842313819 | |

| 49 h | 6.23361425363144 | 4.08843252368054 | 0.23095818127673 |
|------|--------------------------|--------------------|--------------------|
| 50 h | 5.50342795117758 | 3.79089272276261 | -4.45153252168483 |
| 51 h | 4.51403323849951 | 6.94801868971114 | -4.49357020406755 |
| 52 h | 8.78781051292891 | 8.30144360056448 | -2.91077563930344 |
| 53 h | 9.77599981533583 | 5.14573431359676 | -2.89148582523260 |
| 54 h | 9.07132323465438 | 4.89962179446485 | -7.57375291094819 |
| 55 h | 8.08657709225081 | 8.05583916857271 | -7.58942325320918 |
| 56 h | 12.34233718845234 | 9.38742894874678 | -5.98874185062251 |
| 57 h | 13.32573047662530 | 6.23294838453822 | -5.98230884058579 |
| 58 h | 14.84068131382013 | 8.42615121454805 | -9.87368471034062 |
| 59 h | 12.69807446450353 | 6.01549557401042 | -10.70183208317628 |
| 60 h | 11.70974426861233 | 9.19497966816740 | -10.70681072987848 |
| 61 h | -6.37556087340909 | 11.93068963249811 | 0.05665762026752 |
| 62 h | -5.19741249778299 | -3.58835684524685 | 2.91607513417198 |
| 63 h | -7.35810277388803 | -7.63746482498102 | 3.25103171703421 |
| 64 h | -1.84064214629956 | -11.02702488398721 | -1.61473594061432 |
| 65 h | 0.27656085342643 | -6.95760530558506 | -2.01125131948506 |
| 66 h | -7.86444962927714 | -11.61671611389830 | 2.43097463284157 |
| 67 h | -14.34902590005350 | 5.94964891231903 | 1.45081103466884 |
| 68 h | -3.69697094149628 | -19.42702329292126 | -2.36824593812330 |
| 2.3 | Cartesian coordinates of | the E_3 dye | |
| ATOM | CARTESI | AN COORDINATES | |
| 1 c | -0.02329286264356 | -2.12661147555771 | -0.22905630070272 |
| 2 c | 2.63075209586110 | -1.98553575946069 | -0.04173873612884 |
| 3 c | 3.90311581053627 | 0.29311499540992 | 0.16474562486037 |
| 4 c | 2.47569954182495 | 2.50163855659965 | 0.18909175695543 |
| 5 c | -0.18623650390670 | 2.42327441097187 | 0.00700143895919 |
| 6 c | -1.41920555358116 | 0.11687907480319 | -0.20502140949094 |

| 7 n | 3.25593505811093 | 5.00600878541846 | 0.36207369899040 |
|------|--------------------|--------------------|-------------------|
| 8 c | 1.15862390234149 | 6.53508704018710 | 0.32356075434110 |
| 9 c | -1.04548437225335 | 5.01977386147593 | 0.09527139637502 |
| 10 c | 0.98646842002986 | 9.16732314549321 | 0.46097721331926 |
| 11 c | -1.38774502346367 | 10.22780472175068 | 0.35113034431368 |
| 12 c | -3.63691386614277 | 8.76741678635513 | 0.10958006291422 |
| 13 c | -3.41221711803903 | 6.11766111869873 | -0.01502209940998 |
| 14 c | 5.85409303128863 | 5.84816834882927 | 0.66873602438672 |
| 15 c | 6.70010889991543 | 6.01491310991209 | 3.43116253513591 |
| 16 c | 9.43944652510121 | 6.89326027221038 | 3.68925330885462 |
| 17 c | 10.32629394809580 | 7.09568558173674 | 6.43305040431585 |
| 18 c | 13.06885526415840 | 7.96671905147190 | 6.69536831015850 |
| 19 c | 13.94221045118735 | 8.17271243988084 | 9.43956323847614 |
| 20 c | -5.93831000356291 | 10.21029944298747 | 0.02229053767880 |
| 21 c | -1.29841779009250 | -4.59786845953785 | -0.45307741442577 |
| 22 c | -3.54864513469180 | -4.86058752343486 | -1.83071255063430 |
| 23 c | -4.73091004748954 | -7.17412182933791 | -2.02964674403143 |
| 24 c | -3.74061337249307 | -9.36868153582899 | -0.87660464435595 |
| 25 c | -1.48178501073604 | -9.09727102694977 | 0.50705286367226 |
| 26 c | -0.31245478107944 | -6.77187588968283 | 0.70349963438219 |
| 27 c | -5.19841715827436 | -11.64181581412578 | -1.26221391478843 |
| 28 c | -8.48503501037901 | 9.78874074243715 | -0.19767686475556 |
| 29 c | -10.02809780471769 | 12.14809079500420 | -0.16120223144711 |
| 30 n | -12.62626995792466 | 11.83843877833230 | -0.37391874156923 |
| 31 c | -13.94199231563554 | 9.60243285885122 | -0.62094539634569 |
| 32 n | -12.41769096475085 | 7.48536334067259 | -0.65316744601881 |
| 33 c | -9.79560615248272 | 7.35291532950665 | -0.46349149741380 |
| 34 o | -8.81795346459029 | 5.26718219145562 | -0.53525792344224 |

| 35 o | -9.17098089678466 | 14.27034357000903 | 0.04052810760292 |
|------|--------------------|--------------------|-------------------|
| 36 o | -16.21929235212314 | 9.50059301996030 | -0.79537402708532 |
| 37 c | -5.08072796241841 | -14.14371539442468 | -0.63122136773656 |
| 38 c | -7.24539865668170 | -15.66699799834658 | -1.61544488502677 |
| 39 n | -7.21309195329456 | -18.22699728347018 | -1.04340337986747 |
| 40 c | -5.40880507859360 | -19.52754793036623 | 0.31624235227874 |
| 41 n | -3.45431670862288 | -18.02819035608568 | 1.17557097180256 |
| 42 c | -3.11131383839922 | -15.43904760826971 | 0.85082103707011 |
| 43 o | -8.98395731638681 | -14.81802312551774 | -2.85159075077208 |
| 44 o | -5.52551017361676 | -21.77407098937059 | 0.72093057214027 |
| 45 o | -1.24888804426201 | -14.46939852369615 | 1.79061855867473 |
| 46 h | 3.72317901350129 | -3.71031767696549 | -0.10928380156636 |
| 47 h | 5.94240824855097 | 0.32277107654985 | 0.28901978736160 |
| 48 h | -3.46017971550335 | 0.06138410879465 | -0.29973745324274 |
| 49 h | 2.64144370013097 | 10.34872697742784 | 0.65181645364855 |
| 50 h | -1.56221883481685 | 12.26288549687522 | 0.45474456675331 |
| 51 h | -5.09662385747932 | 4.98945117938775 | -0.19777283540134 |
| 52 h | 7.06723114089827 | 4.55008093668058 | -0.37785632694795 |
| 53 h | 6.03804334253202 | 7.68487445316350 | -0.25037855268128 |
| 54 h | 5.44526184886323 | 7.31000382291538 | 4.44033787426563 |
| 55 h | 6.46498395229671 | 4.16453752798095 | 4.32055044827086 |
| 56 h | 10.67891009098650 | 5.58758334778054 | 2.66640095075239 |
| 57 h | 9.66084622845649 | 8.73235561105581 | 2.76406051579329 |
| 58 h | 9.09233623338363 | 8.40707232756469 | 7.45453128615047 |
| 59 h | 10.10156446273497 | 5.25979768319560 | 7.36278516073888 |
| 60 h | 14.29977250469676 | 6.65284055801637 | 5.67661044996342 |
| 61 h | 13.29227971820820 | 9.79858641076875 | 5.76075046079988 |
| 62 h | 15.90392979551072 | 8.79487838637145 | 9.55963738230358 |

| 63 h | 12.79182619622027 | 9.52656982793962 | 10.49029742311042 |
|------|--------------------|--------------------|-------------------|
| 64 h | 13.80268177262608 | 6.35517657570974 | 10.40775259082375 |
| 65 h | -5.58067003236515 | 12.22516172110070 | 0.17506347171737 |
| 66 h | -4.34853178739672 | -3.24446269229936 | -2.79125962167726 |
| 67 h | -6.45799614411685 | -7.32161153031234 | -3.11580701274986 |
| 68 h | -0.68290062871639 | -10.72565540034710 | 1.42829099116029 |
| 69 h | 1.38781224189880 | -6.62695437329622 | 1.82783555304103 |
| 70 h | -6.87976380919452 | -11.27992745907902 | -2.38188514116810 |
| 71 h | -13.67436163336659 | 13.43217075198526 | -0.34580035246908 |
| 72 h | -13.32243179890446 | 5.81497187805708 | -0.83099957544585 |
| 73 h | -8.67294596946460 | -19.26196973733830 | -1.70480334665940 |
| 74 h | -2.10687292918553 | -18.92285004316167 | 2.18777542739741 |

2. Spectral characterization of dyes and their intermediates



Fig S1: ¹H NMR spectrum of intermediate 3





Fig S3: ¹H NMR spectrum of intermediate 4



Fig S4: ¹³C NMR spectrum of intermediate 4



Fig S5: TOF-HRMS spectrum of intermediate 4



Fig S6: ¹H NMR spectrum of E_1



Fig S7: ¹³C NMR spectrum of E_1



Fig S9: ¹H NMR spectrum of E_2



Fig S10: ¹³C NMR spectrum of E_2



Fig S11: ESI-MS spectrum of E_2



Fig S12: ¹H NMR spectrum of E₃



Fig S13: ¹³C NMR spectrum of E₃



Fig S14: ESI-MS of E₃

3. CV studies

The CV measurements were performed on an Ivium Vertex electrochemical workstation by using the three electrode system, consisting of dye casted on glassy carbon electrode as the working electrode, Pt electrode as a counter and Ag/AgCl as a reference electrode. All three electrodes were immersed in the acetonitrile solution consisting 0.1 M tetrabutyl ammonium hexafluorophosphate as supporting electrolyte and data were recorded at a scan rate of 100 mV/s. The obtained CV traces of E_{1-3} are presented in Fig S15 and the corresponding values are summarized in Table 1.



4. Device fabrication and photovoltaic studies

4.1 Photoelectrochemical measurements

Photocurrent-voltage characteristics of DSCs were measured using a Keithley 2400 source meter under illumination of AM 1.5 G solar light from solar simulator (SOL3A, Oriel) equipped with a 450 W xenon lamp (91160, Oriel). The incident light intensity was calibrated using a reference Si solar cell (Newport Oriel, 91150V) to set 1 Sun (100 mW/cm²). The measurement was fully controlled under Oriel IV Test Station software.

IPCE (incident monochromatic photon to current conversion efficiency) experiments were carried out using a system (QEX10, PV Measurements, USA) equipped with a 75 W short arc xenon lamp (UXL-75XE, USHIO, Japan) as a light source connected to a monochromater. Calibration of incident light was performed before measurements using a silicone photodiode (IF035, PV Measurements). All the measurements were carried out without the use of anti-reflecting film.

The electrochemical impedance spectroscopy measurements were performed to understand carrier transportation behavior and interfacial charge recombination processes in fabricated DSSCs. Currently, EIS analysis is one of the most powerful techniques used to obtain additional information, mainly interfacial reactions of photoexcited electrons in DSSCs ²⁹⁻³⁰. In the present study, EIS spectra were recorded over a frequency range of 100 mHz to 200 kHz at 298K with the Bio-Logic SP-150 impedance analyzer under the illumination under solar illumination using a solar simulator (SOL3A, Oriel) equipped with a 450 W xenon lamp (91160, Oriel). The applied voltage was set at the V_{OC} of the DSSCs with AC amplitude fixed at 10 mV. The resultant plots were fitted *via* Z-Fit software (Bio-Logic).

4.2 TiO₂ electrode preparation and device fabrication

Fluorine-doped tin oxide (FTO) coated glasses (2.2 mm thickness, sheet resistance of 8 Ω /cm², TEC, Pilkington) were washed with detergent, water, acetone and ethanol, sequentially. After this FTO glass plates were immersed into a 40 mM aqueous TiCl₄ solution at 70 °C for 30 min and washed with water and ethanol. Thin layer (8-12 µm thick) of TiO₂ (Solaronix, Ti-Nanoxide D/SP) was deposited (active area, 0.18 cm²) on transparent conducting glass by squeegee printing followed by drying at 350 °C for 10 min and curing at 500 °C for 30 min. Next, after drying the electrodes, scattering layer (5 µm thick) TiO₂ particles (Solaronix, Ti-Nanoxide R/SP) were printed

onto the already deposited TiO₂ layer. The TiO₂ electrodes were heated under an air flow at 350 °C for 10 min, followed by heating at 500 °C for 30 min. After cooling to room temperature, the TiO₂ electrodes were treated with 40 mM aqueous solution of TiCl₄ at 70 °C for 30 min and then washed with water and ethanol. The electrodes were heated again at 500 °C for 30 min and left to cool to 80 °C before dipping them into the dye solution. The dye solutions (0.3 mM) were prepared in 10 mL 1:1:1 acetonitrile, *tert*-butanol and dimethyl sulfoxide. Chenodeoxycholic acid (CDCA) was added at a concentration of 10 mM. The electrodes were immersed in the dye solutions and then kept at 25 °C for 20 hours to adsorb the dye onto the TiO₂ surface.

For preparing the counter electrode, pre-cut TCO glasses were washed with water followed by 0.1M HCl in EtOH, and sonication in acetone bath for 10 min. These washed TCO were then dried at 400 °C for 15 min. Thin layer of Pt-paste (Solaronix, Platisol T/SP) on TCO was printed and the printed electrodes were then cured at 450 °C for 10 min. The dye sensitized TiO₂ electrodes were sandwiched with Pt counter electrodes and the electrolyte (Solaronix, Iodolyte HI-30) was then injected into the cell, while the two electrodes were held together with the clips.

4.3 TiO₂ electrode preparation and device fabrication for co-sensitized devices

Fluorine-doped tin oxide (FTO) coated glasses (2.2 mm thickness, sheet resistance of 8 Ω /cm², TEC, Pilkington) were washed with detergent, water, acetone and ethanol, sequentially. After this FTO glass plates were immersed into a 40 mM aqueous TiCl₄ solution at 70 °C for 30 min and washed with water and ethanol. Thin layer (8-12 µm thick) of TiO₂ (Solaronix, Ti-Nanoxide D/SP) was deposited (active area, 0.18 cm²) on transparent conducting glass by squeegee printing followed by drying at 350 °C for 10 min and curing at 500 °C for 30 min. Next, after drying the electrodes, scattering layer (5 µm thick) TiO₂ particles (Solaronix, Ti-Nanoxide R/SP) were printed onto the already deposited TiO₂ layer. The TiO₂ electrodes were heated under an air flow at 350 °C for 10 min, followed by heating at 500 °C for 30 min. After cooling to room temperature, the TiO₂ electrodes were treated with 40 mM aqueous solution of TiCl₄ at 70 °C for 30 min and then washed with water and ethanol. The electrodes were heated again at 500 °C for 30 min and left to cool to 80 °C before dipping them into the dye solution. The dye solutions were prepared in 10 mL 1:1:1 acetonitrile, *tert*-butanol and dimethyl sulfoxide, and **NCSU-10** and **E**₁₋₃ were then dissolved based on the required concentration. Chenodeoxycholic acid (CDCA) was added at a

concentration of 10 mM. The electrodes were immersed in the dye solutions and then kept at 25 $^{\circ}$ C for 20 hours to adsorb the dye onto the TiO₂ surface.

For preparing the counter electrode, pre-cut TCO glasses were washed with water followed by 0.1M HCl in ethanol, and sonication in acetone bath for 10 min. These washed TCO were then dried at 400 °C for 15 min. Thin layer of Pt-paste (Solaronix, Platisol T/SP) on TCO was printed and the printed electrodes were then cured at 450 °C for 10 min. The dye sensitized TiO_2 electrodes were sandwiched with Pt counter electrodes and the electrolyte (Solaronix, Iodolyte HI-30) was then injected into the cell, while the two electrodes were held together with the clips.