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

Supporting Information

for

Exploring ultrafast dynamics of diarylethene derivative by sub-10 fs laser pulses

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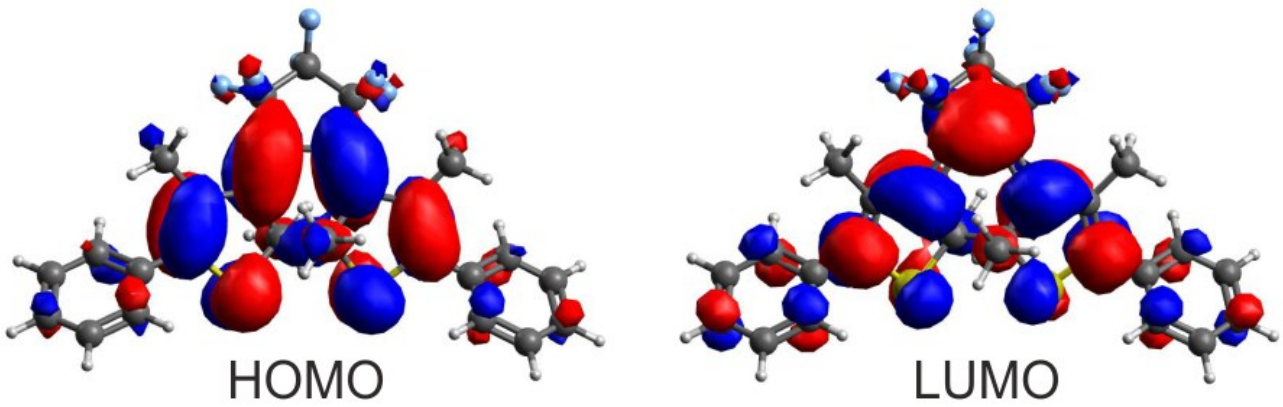

Fig. S1. The NTO orbitals of HOMO and LUMO of DMP closed isomer.

Geometries of the DMP molecule optimized at B3LYP/6-31G* level.
XYZ coordinates given in Å

1. The ground state minimum

```
C1 -1.4430520000  0.4155900000-0.1823070000
C2 -0.6131300000 -0.8705600000 -0.3205410000
C3  0.6513070000 -0.7732110000 0.5578920000
S4  1.7984730000 -2.2236050000 0.3607900000
C5 -0.7306590000  1.5810500000 -0.1110640000
C6 -1.2477780000  2.9933840000 -0.1337990000
C7  0.7335710000  1.5977320000 -0.0665860000
C8 -0.0164660000  3.8722580000 0.2010010000
C9  1.2124870000  3.0156220000 -0.1974830000
F10 -2.2489290000 3.2427830000 0.7586910000
F11 -1.7175260000 3.3599370000 -1.3708840000
F12 -0.0440750000 5.0668180000 -0.4212630000
F13  0.0204290000 4.0785440000 1.5424310000
F14  1.5801680000 3.3425560000 -1.4804780000
F15  2.2636290000 3.3351280000 0.6087220000
C16  1.4665000000 0.4540260000 0.1151340000
C17  0.3559730000 -0.6325660000 2.0740050000
H18  1.2996490000 -0.5213360000 2.6119170000
H19 -0.1647720000 -1.5101740000 2.4593300000
H20 -0.2581520000  0.2508200000 2.2638330000
C21 -0.3077640000 -1.0674070000 -1.8291090000
H22  0.2310370000 -1.9994330000 -2.0035440000
H23  0.2922380000 -0.2364840000 -2.2097250000
H24 -1.2486350000 -1.0954280000 -2.3824830000
C25  3.1847590000 -1.1507910000 0.1090650000
S26 -1.7668060000 -2.2310430000 0.2078570000
C27 -3.1707730000 -1.1712740000 -0.0296170000
C28 -4.5022090000 -1.8034960000 0.0242660000
C29 -5.5530670000 -1.2145890000 0.7512690000
C30 -4.7402710000 -3.0312420000 -0.6217240000
C31 -6.8050840000 -1.8232040000 0.8113130000
H32 -5.3767880000 -0.2912210000 1.2918630000
C33 -5.9946380000 -3.6334000000 -0.5642390000
H34 -3.9383600000 -3.5016730000 -1.1814510000
C35 -7.0325790000 -3.0315650000 0.1509450000
H36 -7.6013200000 -1.3560550000 1.3831160000
H37 -6.1617740000 -4.5748320000 -1.0789710000
H38 -8.0088680000 -3.5045940000 0.1987160000
C39 -2.8688970000  0.1534820000 -0.2319650000
C40 -3.9052840000  1.2055410000 -0.5400960000
H41 -4.8343410000  0.7442680000 -0.8782690000
H42 -4.1299430000  1.8290920000 0.3302760000
H43 -3.5474710000  1.8762720000 -1.3237530000
C44  4.5122840000 -1.7870320000 0.0325970000
C45  5.6152550000 -1.2459250000 0.7181810000
C46  4.6951120000 -2.9747510000 -0.6995970000
C47  6.8627160000 -1.8637130000 0.6569970000
H48  5.4836560000 -0.3531420000 1.3200060000
C49  5.9443220000 -3.5868330000 -0.7619270000
H50  3.8550620000 -3.4056130000 -1.2357110000
C51  7.0329620000 -3.0333360000 -0.0854690000
H52  7.7007460000 -1.4345050000 1.1979830000
H53  6.0678570000 -4.4971230000 -1.3409690000
H54  8.0057600000 -3.5133950000 -0.1320280000
C55  2.8808080000  0.1850230000 -0.0109010000
C56  3.8967730000  1.2264730000 -0.4097370000
H57  3.4901720000  1.8710980000 -1.1929020000
H58  4.1725370000  1.8778660000 0.4241600000
H59  4.8027050000  0.7563420000 -0.7937330000
```

2. The S_1 state minimum

```
C1 -1.4263070000 0.4174960000 -0.3135810000
C2 -0.5707850000 -0.8330810000 -0.4217280000
C3 0.6233200000 -0.7216490000 0.6231280000
S4 1.7679300000 -2.1591120000 0.5914950000
C5 -0.7019240000 1.6275080000 -0.1977970000
C6 -1.2414970000 3.0278780000 -0.1751720000
C7 0.7091700000 1.6501020000 -0.0361900000
C8 -0.0349760000 3.9155280000 0.2273560000
C9 1.2102130000 3.0579720000 -0.0963330000
F10 -2.2606020000 3.2149530000 0.7190050000
F11 -1.7177190000 3.4385010000 -1.3960750000
F12 -0.0348360000 5.1048680000 -0.4092810000
F13 -0.0724550000 4.1444190000 1.5651540000
F14 1.6693790000 3.4151560000 -1.3480670000
F15 2.2209730000 3.3305020000 0.7771290000
C16 1.4601500000 0.4694240000 0.1930710000
C17 0.1011410000 -0.5697080000 2.0704720000
H18 0.9416880000 -0.4392920000 2.7572280000
H19 -0.4654810000 -1.4555590000 2.3714090000
H20 -0.5511750000 0.3050370000 2.1447590000
C21 -0.0479470000 -1.0062560000 -1.8671010000
H22 0.5403430000 -1.9250230000 -1.9536520000
H23 0.5774660000 -0.1546240000 -2.1500190000
H24 -0.8920080000 -1.0634760000 -2.5594850000
C25 3.1628490000 -1.1646240000 0.1792220000
S26 -1.7086980000 -2.2364430000 -0.0591270000
C27 -3.1365820000 -1.2026480000 -0.1534370000
C28 -4.4450700000 -1.8411240000 -0.0316900000
C29 -5.5139020000 -1.2173150000 0.6503400000
C30 -4.6652700000 -3.1359130000 -0.5540890000
C31 -6.7457380000 -1.8512780000 0.7821890000
H32 -5.3624970000 -0.2481190000 1.1116930000
C33 -5.8984700000 -3.7653050000 -0.4170150000
H34 -3.8667750000 -3.6352150000 -1.0951050000
C35 -6.9480930000 -3.1262840000 0.2475000000
H36 -7.5481250000 -1.3519700000 1.3187800000
H37 -6.0428980000 -4.7568530000 -0.8377430000
H38 -7.9108820000 -3.6184320000 0.3527820000
C39 -2.8243270000 0.1521720000 -0.3145320000
C40 -3.8861050000 1.2017510000 -0.5404380000
H41 -4.7889170000 0.7471880000 -0.9546910000
H42 -4.1613810000 1.7228770000 0.3826560000
H43 -3.5324490000 1.9600580000 -1.2409260000
C44 4.4596490000 -1.8196940000 0.0614760000
C45 5.6503390000 -1.1836480000 0.4827350000
C46 4.5610790000 -3.1384300000 -0.4396180000
C47 6.8789170000 -1.8296690000 0.3849800000
H48 5.6016120000 -0.1948840000 0.9251930000
C49 5.7921810000 -3.7775240000 -0.5346730000
H50 3.6653350000 -3.6497580000 -0.7810350000
C51 6.9605610000 -3.1272090000 -0.1272320000
H52 7.7772920000 -1.3206960000 0.7241320000
H53 5.8414810000 -4.7867140000 -0.9348700000
H54 7.9216260000 -3.6281260000 -0.2014170000
C55 2.8320730000 0.1863770000 -0.0088880000
C56 3.8240510000 1.2009690000 -0.5221450000
H57 3.3502050000 1.8694270000 -1.2438690000
H58 4.2159950000 1.8317770000 0.2835940000
H59 4.6669750000 0.7107630000 -1.0129610000
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3. The structure in the vicinity of the conical intersection

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C1 -1.4333900000 0.4169100000 -0.3792000000
C2 -0.6393000000 -0.8011500000 -0.6289300000
C3 0.7036500000 -0.6826000000 0.8215200000
S4 1.7970100000 -2.0786100000 0.8929500000
C5 -0.6930500000 1.6237900000 -0.2505400000
C6 -1.2186700000 3.0339000000 -0.2288500000
C7 0.6882500000 1.6299900000 -0.0107000000
C8 -0.0104100000 3.9073000000 0.2077700000
C9 1.2243600000 3.0256900000 -0.0849100000
F10 -2.2410400000 3.2328700000 0.6546200000
F11 -1.6682100000 3.4600600000 -1.4542300000
F12 0.0266000000 5.1042600000 -0.4137300000
F13 -0.0765900000 4.1218400000 1.5472600000
F14 1.7020000000 3.3404900000 -1.3381600000
F15 2.2322000000 3.2999300000 0.7927900000
C16 1.4465600000 0.4253100000 0.2318900000
C17 -0.1459700000 -0.4945100000 2.0669100000
H18 0.5034200000 -0.2911500000 2.9257600000
H19 -0.7285000000 -1.3957300000 2.2772500000
H20 -0.8250600000 0.3475100000 1.9370500000
C21 0.1908300000 -0.9426600000 -1.9017900000
H22 0.7580000000 -1.8772200000 -1.9091400000
H23 0.8816800000 -0.1047200000 -2.0089400000
H24 -0.4812800000 -0.9447100000 -2.7674800000
C25 3.1606900000 -1.1690700000 0.2554200000
S26 -1.7071500000 -2.1987400000 -0.3724400000
C27 -3.1501000000 -1.1924700000 -0.2037300000
C28 -4.4491000000 -1.8462400000 -0.0376000000
C29 -5.3947000000 -1.3719700000 0.8946400000
C30 -4.7793400000 -2.9911000000 -0.7919000000
C31 -6.6261700000 -2.0040600000 1.0486400000
H32 -5.1470700000 -0.5163300000 1.5148700000
C33 -6.0100900000 -3.6227100000 -0.6319500000
H34 -4.0669800000 -3.3723200000 -1.5179800000
C35 -6.9409100000 -3.1311800000 0.2859500000
H36 -7.3373100000 -1.6226100000 1.7766000000
H37 -6.2456800000 -4.4981700000 -1.2313200000
H38 -7.9011700000 -3.6245500000 0.4089900000
C39 -2.8375800000 0.1674300000 -0.2636000000
C40 -3.9318900000 1.2063700000 -0.3105300000
H41 -4.8652400000 0.7391800000 -0.6327800000
H42 -4.1097000000 1.6779600000 0.6609200000
H43 -3.6840700000 2.0029800000 -1.0139200000
C44 4.4500900000 -1.8439100000 0.1089600000
C45 5.6415400000 -1.2328400000 0.5479000000
C46 4.5271400000 -3.1383200000 -0.4432000000
C47 6.8639100000 -1.8882600000 0.4211600000
H48 5.6001400000 -0.2519200000 1.0107900000
C49 5.7510500000 -3.7899200000 -0.5642500000
H50 3.6198800000 -3.6237200000 -0.7923100000
C51 6.9262600000 -3.1674100000 -0.1358800000
H52 7.7701200000 -1.4009500000 0.7707200000
H53 5.7881700000 -4.7844800000 -1.0003400000
H54 7.8812200000 -3.6763500000 -0.2313300000
C55 2.8117400000 0.1557600000 -0.0271500000
C56 3.7658900000 1.1278700000 -0.6750200000
H57 3.2757000000 1.6750600000 -1.4847800000
H58 4.1193600000 1.8756300000 0.0425500000
H59 4.6345400000 0.6096200000 -1.0863900000
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