*Electronic Supplementary Information (ESI)*

# Enhancing the power conversion efficiency of dye-sensitized solar cells via molecular plasmon-like excitations

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## Contents

## 1. Computational details

Geometries of the known (MK-1, MK-2, MK-3, MK-8, WS-52, and WS-55) and newly designed dyes (MK-2'D, MK-2D, MK-2DBOD, MK-8DBOD etc.) in their (singlet) ground state were optimised in vacuum using DFT/ωB97X-D[1]/6-31G*[2] as implemented in the Q-Chem 4.3 package.[3] The singlet electronic excitation energies and oscillator strengths of the first 6 excitations (10 for MK-8DBOD) of these molecules in the optimized geometries were then computed in vacuum using linear response (LR) TDDFT[4] at the ωB97X-D/cc-pVDZ[5] level. Lorentzian broadening with Γ=0.5 eV was applied to the computed excitations to simulate their absorbance. ωB97X-D/cc-pVTZ geometry optimizations and TD-ωB97X-D/cc-pVTZ absorption spectra were also performed for several molecules to assess the convergence of previous results (Fig. S1). The quality of the LR-TDDFT computations for molecular plasmons has also been examined (Fig. S2). Furthermore, geometry optimizations with DFT/PBE0-D3[6,7]/6-31G followed by TD-ωB97X-D/cc-pVDZ absorption spectra computations were performed for MK-2 and the designed MK-2'D, MK-2'D(CNC, Par, Par), and MK-2DBOD dyes to allow direct comparison with the molecular dynamics (MD) simulations.

The oxidation potentials of the ground state (GSOP) and first singlet excited state (ESOP) of the investigated molecules were estimated by $\varepsilon_{HOMO}$ and $(\varepsilon_{HOMO}+\varepsilon_{S1})$[8] respectively, obtained from TD-ωB97X-D/cc-pVDZ at the ωB97X-D/6-31G* optimized geometries, where $\varepsilon_{S1}$ stands for the vertical first singlet excitation energy.

We also analysed the solvent effect on the molecular properties of interest by using the closely-related conductor-like polarizable continuum model (CPCM)[9-11] implemented in Q-Chem. Tetrahydrofuran (THF) solvent was implicitly added around the MK-2, MK-2'D, and MK-2DBOD for non-equilibrium LR-TDDFT/CPCM computations (by setting the optical dielectric constant) and their absorption spectra are compared to those computed in gas phase as discussed above.

To examine the effects of nuclear thermal motions on the absorption spectra, MD simulations at 300 K were performed for MK-2 and the designed dyes MK-2'D, MK-2'D(CNC, Par, Par), and MK-2DBOD at the PBE0-D3/6-31G level (in vacuum), as implemented in the TeraChem[,12,13] package. In these MD simulations, trajectories were run with the time step of 1 fs; after thermalization, the sampling was initiated at 5000 fs. We sampled geometry per 500 fs until 25 geometries (the final one at 17000 fs) were gathered. The absorption spectra

of these sampled structures were each computed at the TD-ωB97X-D/cc-pVDZ level (Q-Chem), followed by Lorentzian broadening (Γ=0.5 eV) and averaging to obtain simulated collective absorbance at room temperature. In order to probe the absorption properties of molecular plasmons, three excitations of thiophene and bithiophene molecules and six excitations of quaterthiophene and quaterthiophene dimers (Fig. 1b) were computed using ADC(2)[14,15]/cc-pVTZ, as implemented in the MOLPRO[16,17] package. All the molecular structures given in this paper are plotted using GaussView.[18]

## 2. Convergence of LR-TDDFT results with basis set size

Results shown in Fig. S1 demonstrate that for the low-lying plasmonic excitations of interest in the current work, our standard method, namely, TD-ωB97X-D/cc-pVDZ computed at the ωB97X-D/6-31G* optimized geometries, can produce results in excellent agreement with those computed by TD-ωB97X-D/cc-pVTZ at the ωB97X-D/cc-pVTZ optimized geometries.

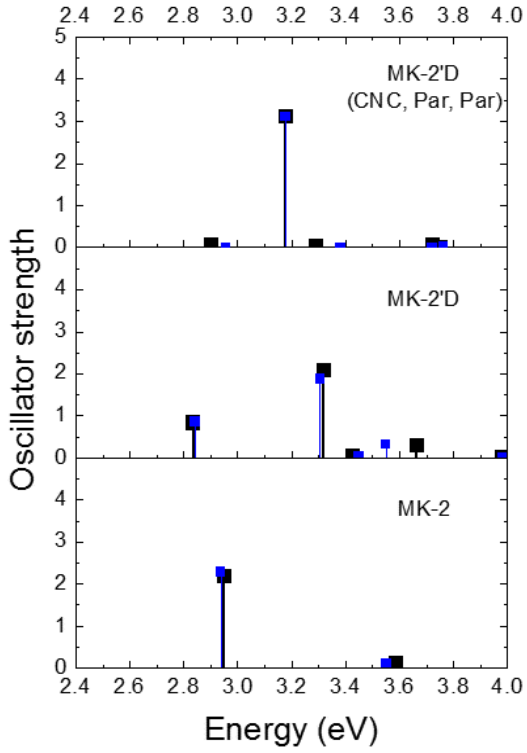



**Fig. S1** TD-ωB97X-D/cc-pVDZ results computed at the ωB97X-D/6-31G* optimized geometries (black squares) in comparison with TD-ωB97X-D/cc-pVTZ results computed at the ωB97X-D/cc-pVTZ optimized geometries (blue squares).

## 3. Quality of LR-TDDFT results on molecular plasmons

Molecular plasmons of octatetraene have been identified to be dominated by single-particle transitions and can be reliably described by LR-TDDFT.[19] Here we compare LR-TDDFT results of bithiophene against those from the high-level method, ADC(3). Clearly, it can be seen in Fig. S2 that the lowest absorption peak (principal peak), which corresponds to the HOMO to LUMO plasmonic excitation (see Fig. 1), is dominated by single-particle transitions and is well described by TD-ωB97X-D.

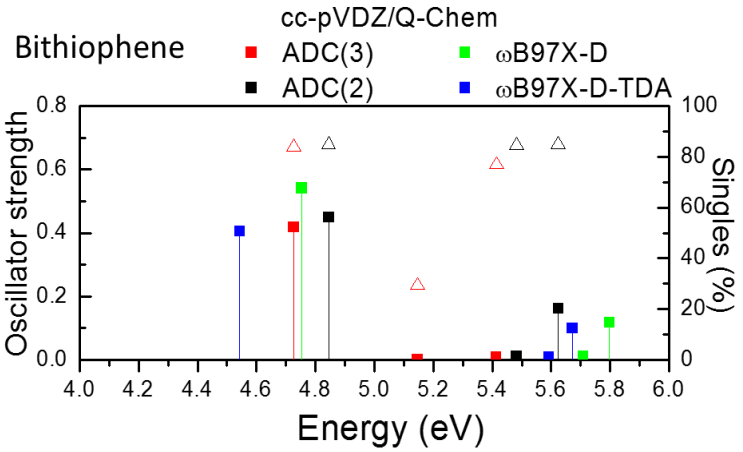



**Fig. S2** The first three electronic excitations of bithiophene computed by various methods: TD-ωB97X-D, TD-ωB97X-D-TDA, ADC(2), and ADC(3). The total contribution of single-particle transitions to each excited state in ADC(2) and ADC(3) computations are also plotted (triangles; right axis). It can be seen that the principal peak is clearly dominated by single-particle transitions.

## 4. Effects of hexyl chains and π-bridge length on the principal absorption peak of MK dyes

We examine the effects of substituting hexyl side-chains and/or adding more thiophene unit(s) to MK dyes. It can be seen in Fig. S3 that lengthening the π-bridge results in a red-shifted absorption energy (MK-3 to MK-1 and MK-2' to MK-2), whereas substituting hexyl chains to a dye can either blue-shift or red-shift the absorption peak (MK-3 to MK-1 and MK-2' to MK-2). The largest observed difference is between the peak of the optimized MK-3 and that of the optimized MK-2' (~0.08 eV). It can be seen that the overall red-shift from the optimized MK-3 to the optimized MK-1 is caused partly by the geometrical difference (black peak to red peak of MK-3) and partly by the electronic structure difference between MK-3 and MK-1.

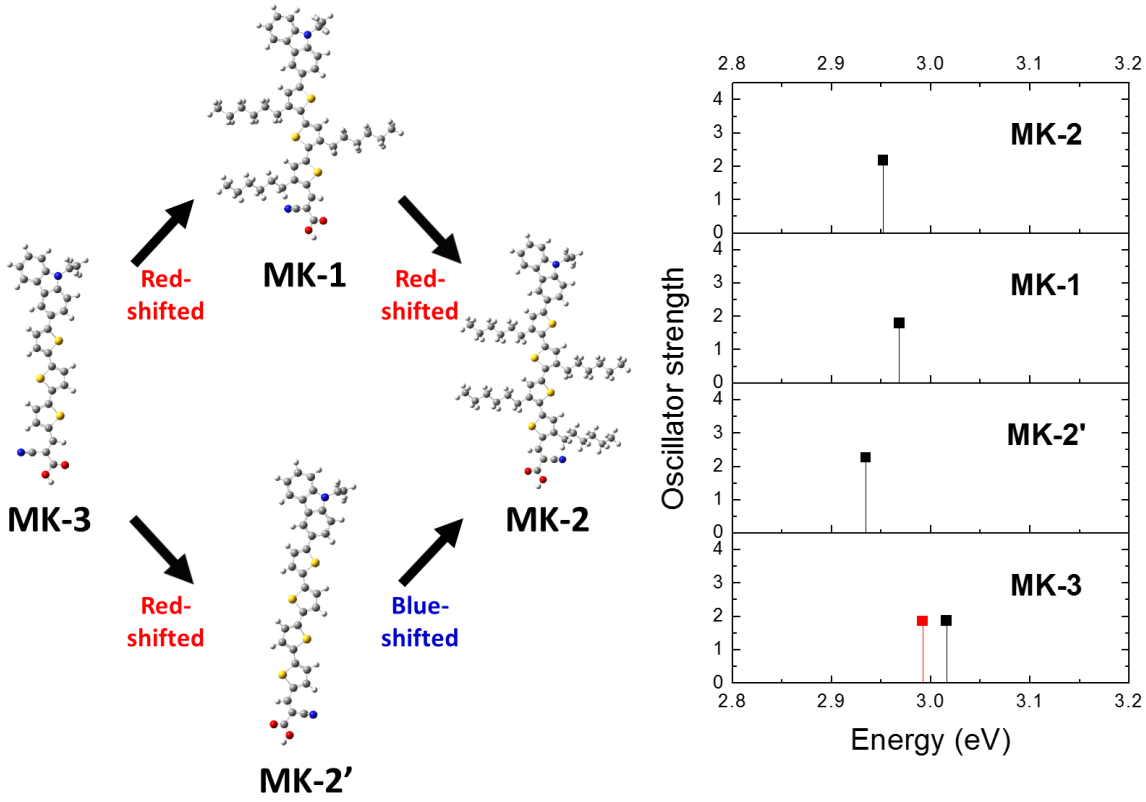



**Fig. S3** Computed excitation energies and oscillator strengths of the principal absorption peaks of geometrically optimized MK-3, MK-1, MK-2, and MK-2' (hexyl side-chains of MK-2 replaced by hydrogens). The red peak corresponds to the principal absorption of MK-3 with the optimized MK-1 geometry (hexyl chains of the optimized MK-1 being replaced by hydrogen atoms).

## 5. Effects of solvent on the absorption spectra of dyes

Although the dielectric effect from solvent can shift the absorption peaks and change the oscillator strengths of the dyes, one expects that the strong absorption feature of the plasmon peaks will remain. In fact, the absorption spectra of MK-3 and MK-2[20] in a working DSSC condition with solvent (THF/toluene=1:4) can be well reproduced by our gas phase computations. This is further demonstrated in Fig. S4 by comparing results with/without the presence of THF solvent, whose dielectric effect is expected to be even more substantial than that of the solvent used in the experiment. Similarly, the presence of triiodide/iodide redox couple in a working DSSC is not expected to qualitatively change the absorption properties of the dyes as in the cases of MK-2 and MK-3 discussed above. Additionally, the hexyl side chains in, for example, MK-2DBOD are expected to reduce the contact between the quaterthiophene unit of the MK-2DBOD and the redox couple.

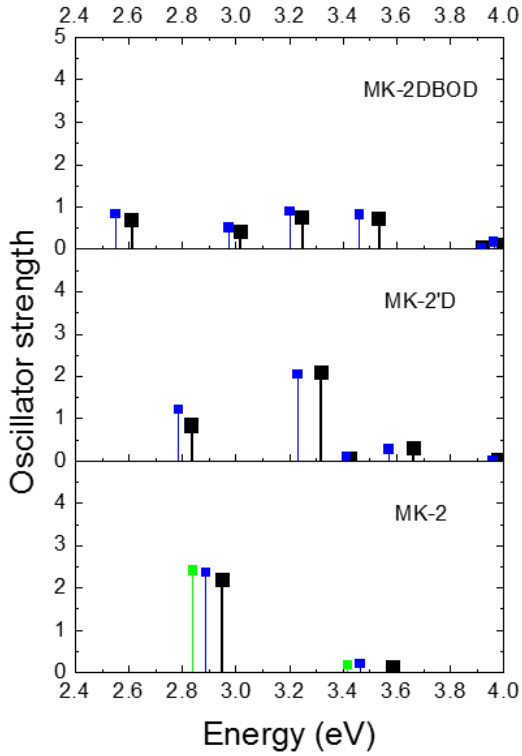



**Fig. S4** Absorption spectra of MK-2, MK-2'D, and MK-2DBOD molecules computed by LR-TDDFT with (blue and green squares) and without (black squares) the presence of the THF solvent. The geometries were optimized in gas phase (blue and black squares) or in THF (green squares).

## 6. Several linkers, which ensure stable π-stacking of dimeric dyes

Several linkers used in forming dimeric dyes are displayed in Fig. S5. The properties of these dyes are discussed in later sections. Note that we do not attempt to optimize the linker group in the present work. Rather, we demonstrated the feasibility of dimeric dye designs using several sensible and 'convenient' linker groups as examples. For instance, the molecular substructures shown in Fig. 5b, where carbazole is substituted by two Sulfur atoms (forming S-C-C-S linker), have been synthesized in the literature.

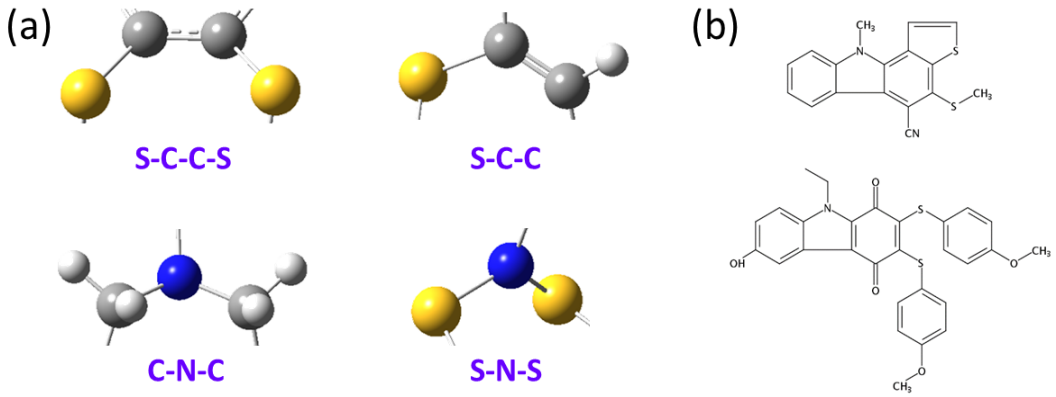



**Fig. S5** (a) Various linkers used in connecting the donor (carbazole) and the two oligothiophene π-conjugated moieties to form dimeric dyes. (b) Molecular substructures, 10*H*-Thieno[3,2-*a*]carbazole-5-carbonitrile, 10-methyl-4-(methylthio)- (above)[21] and 1*H*-Carbazole-1,4(9*H*)-dione, 9-ethyl-6-hydroxy-2,3-bis[(4-methoxyphenyl)thio]- (below)[22], in which the carbazole is substituted by two Sulfur atoms.

## 7. Molecular dynamics of dyes

The structures of the MK-2, MK-2'D, MK-2DBOD, and MK-2'D(CNC, Par, Par) molecules sampled from molecular dynamics are displayed in Fig. S6-S9. The simulated collective absorbances of these molecules at room temperature (obtained from MD simulations) are plotted in Fig. S10, along with the absorption spectra at the optimized geometries.

It can be seen that the broadened absorption feature of the optimized geometries is simply carried to the spectra of the 25 sampled structures (green squares). The thermal effects lead to some variations of the absorbance (red lines vs. green lines); however, the broadened absorbance resulting from plasmons interaction (red and black lines) remains. We also note that the absorption spectra of the MD-simulated structures of MK-2'D(CNC, Par, Par), which has only single-peaked absorption at either ωB97X-D/6-31G* or PBE0+D3/6-31G optimized geometries, is narrower in width compared to those of MK-2'D and MK-2DBOD. This is attributed to the strong distortion of the two π-conjugated moieties of the molecule such that the plasmon interactions the two moieties are weakened.

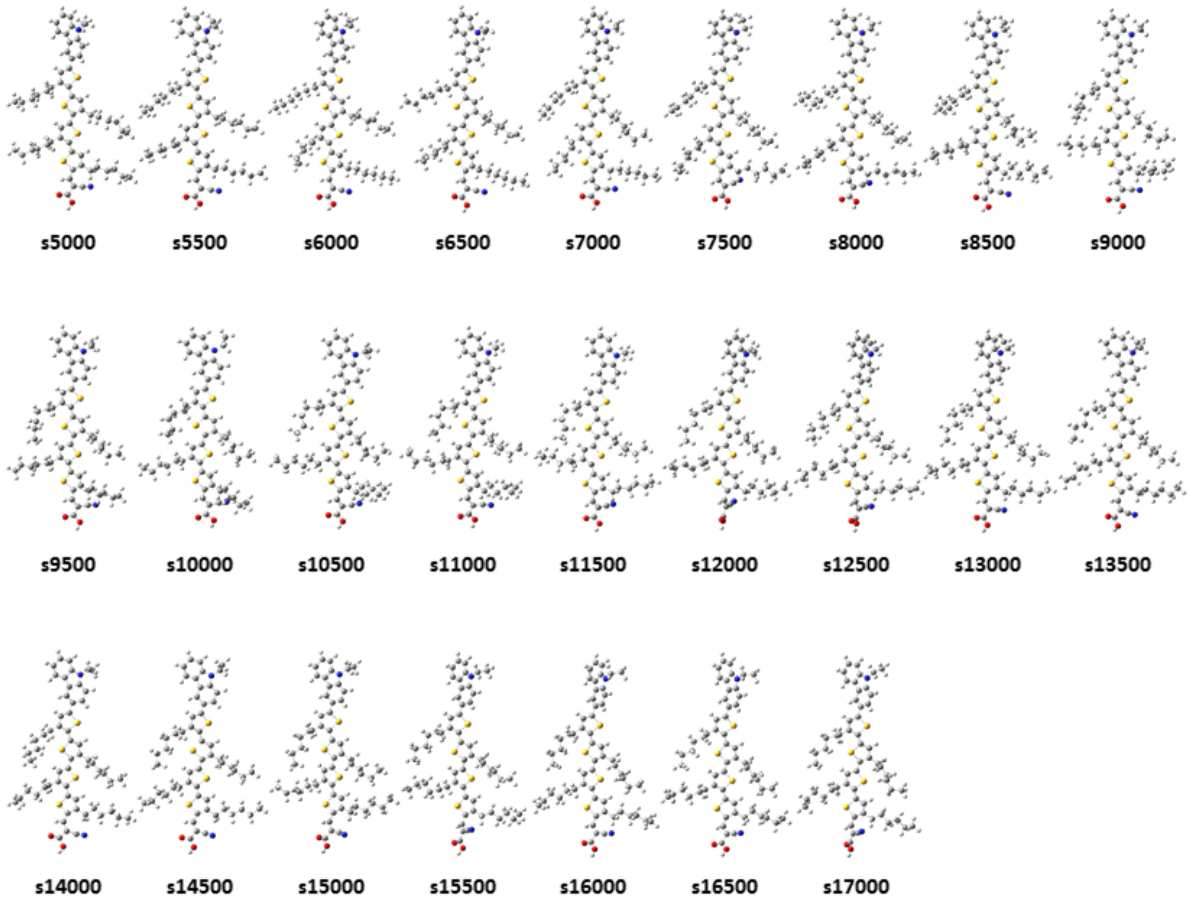



**Fig. S6** MK-2 geometries sampled from the MD simulation. s6500, for example, denotes the time step of 6500 fs in the MD simulation. With the hexyl chains accordingly attached (in contrast to MK-4 and MK-5 for example)[20], the average distance between MK-2 dyes are larger than that of MK-3 on the $TiO_2$ surface.

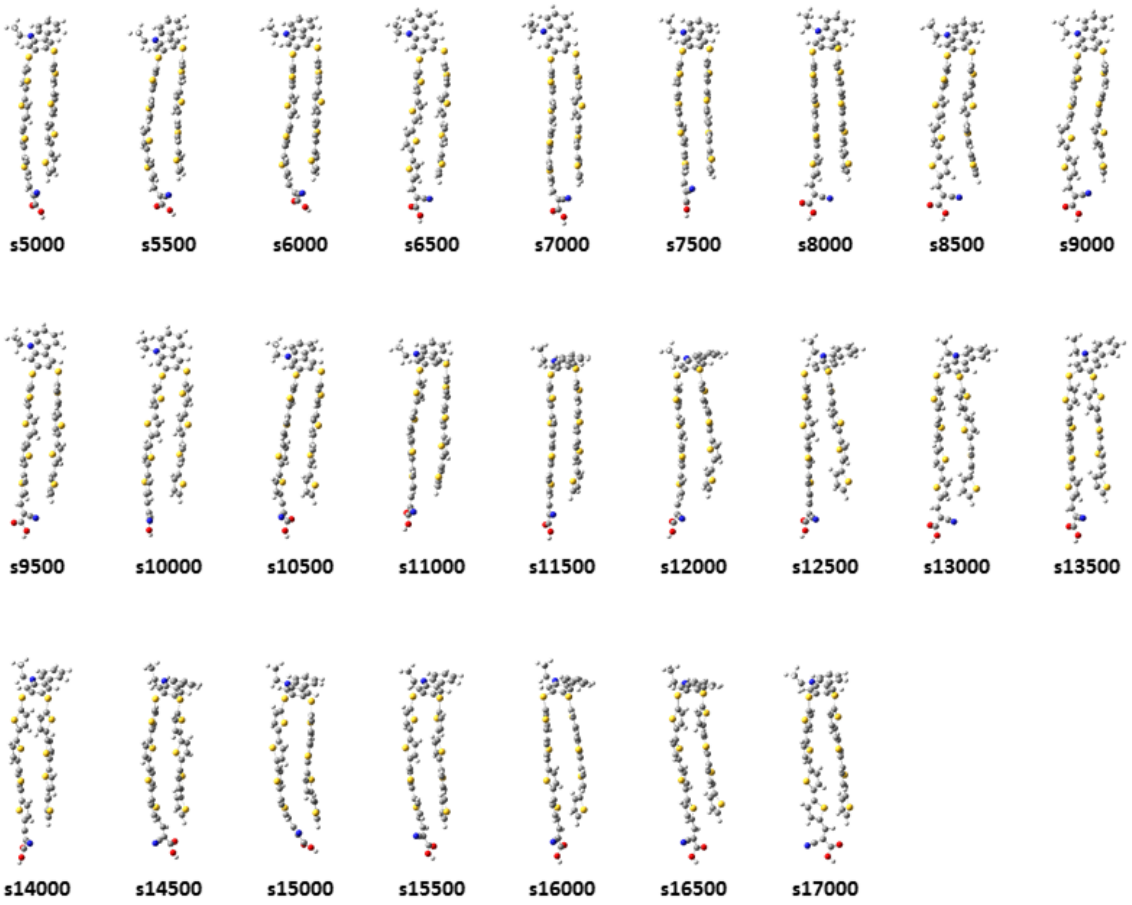



**Fig. S7** MK-2’D geometries sampled from the MD simulation. The π-stacking of the molecule is stable under thermal motions.

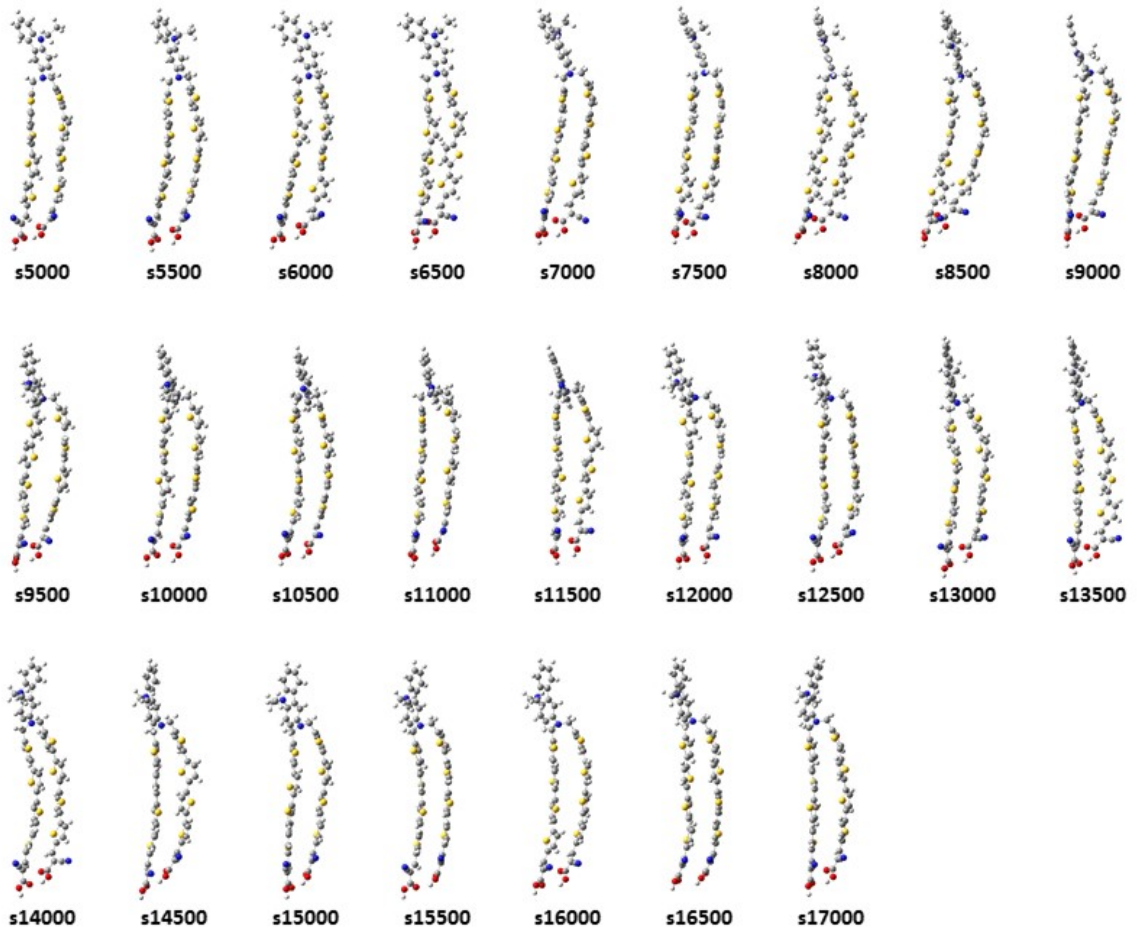



**Fig. S8** MK-2'D(CNC, Par, Par) geometries sampled from the MD simulation. The distortion of the π-conjugated moieties is attributed to the interaction between the two anchoring groups.

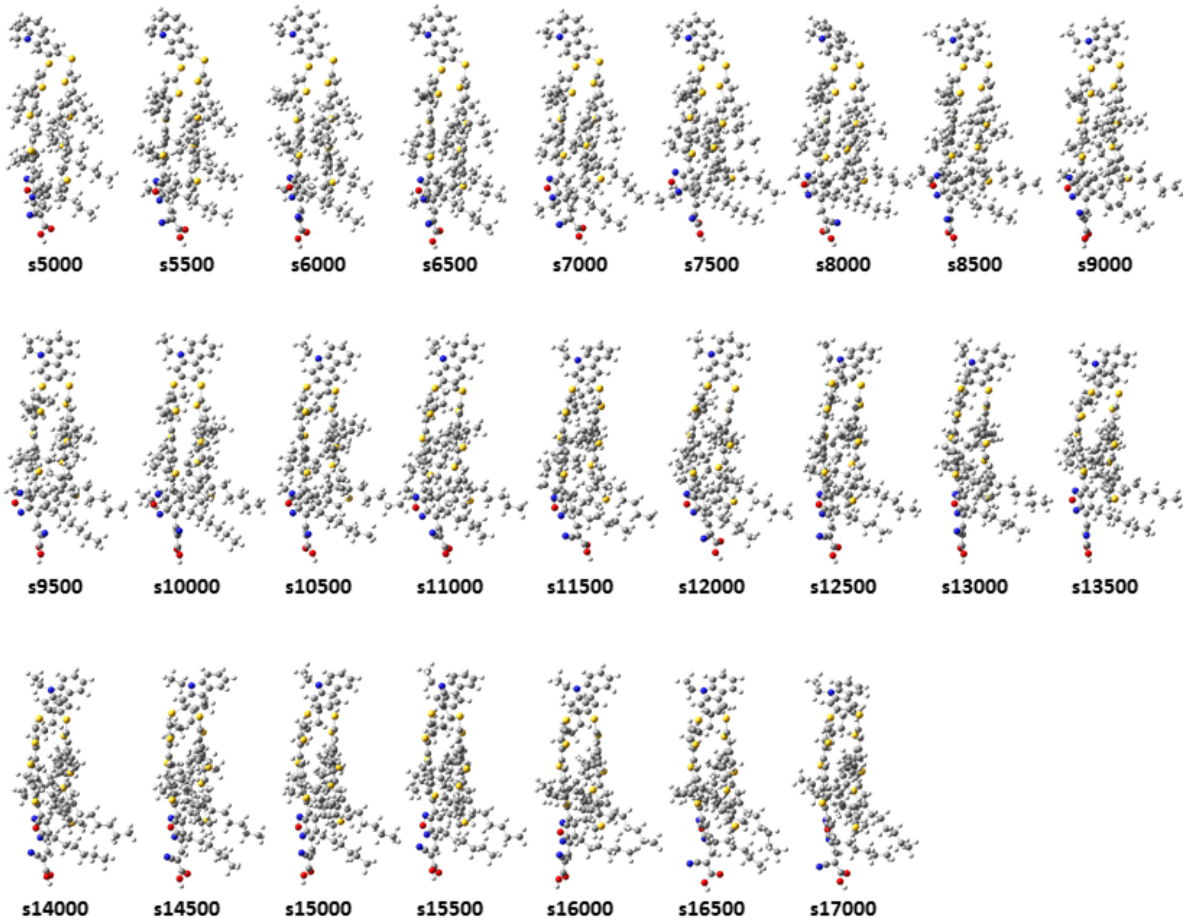



**Fig. S9** MK-2DBOD geometries sampled from the MD simulation. With the presence of hexyl side-chains, the π-stacking of the molecule remains stable under thermal motions. The thermally geometrical fluctuations around the optimized structure (energy minimum) allow a further broadened absorption spectrum (Fig. S10).

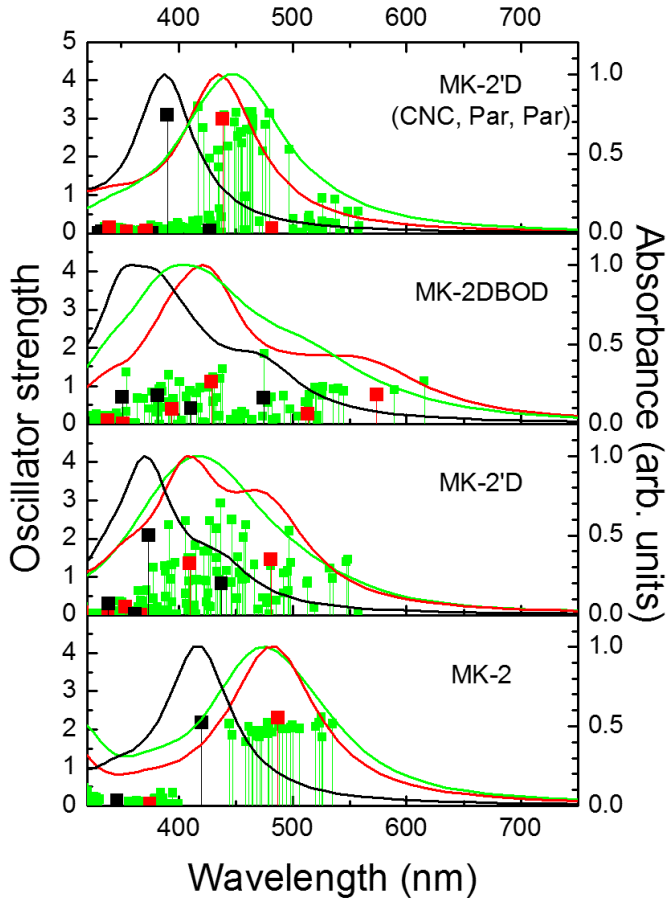
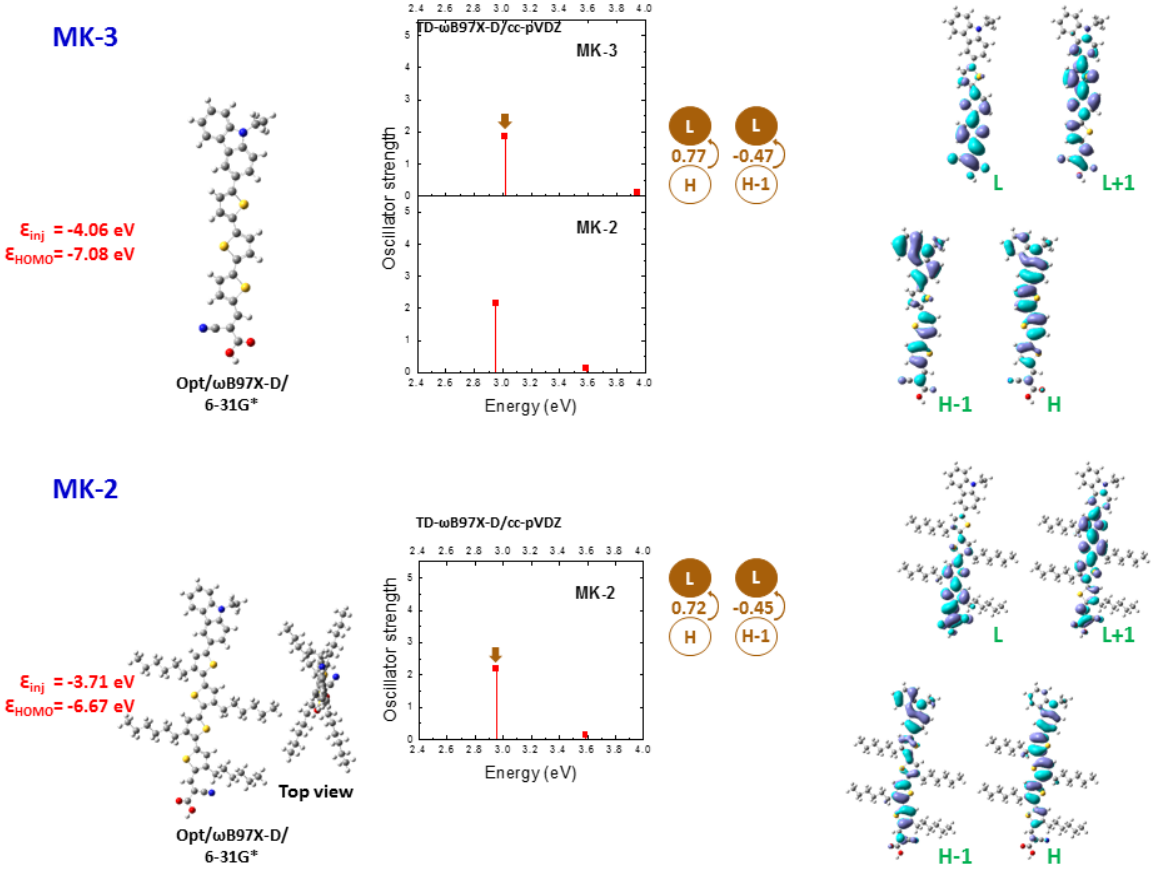



**Fig. S10** Absorption spectra of MK-2, MK-2'D, MK-2DBOD, and MK-2'D(CNC, Par, Par) molecules computed by TD-ωB97X-D/cc-pVDZ at the ωB97X-D/6-31G* optimized geometries (black squares) and at the PBE0+D3/6-31G optimized geometries (red squares). These results are backgrounded by the TD-ωB97X-D/cc-pVDZ results for the MD-sampled 25 structures (green squares). Computed absorbances of these molecules at the ωB97X-D/6-31G* (black lines) and PBE0+D3/6-31G (red lines) optimized structures and the MD-simulated collective absorbances at room temperature (green lines) are also plotted.

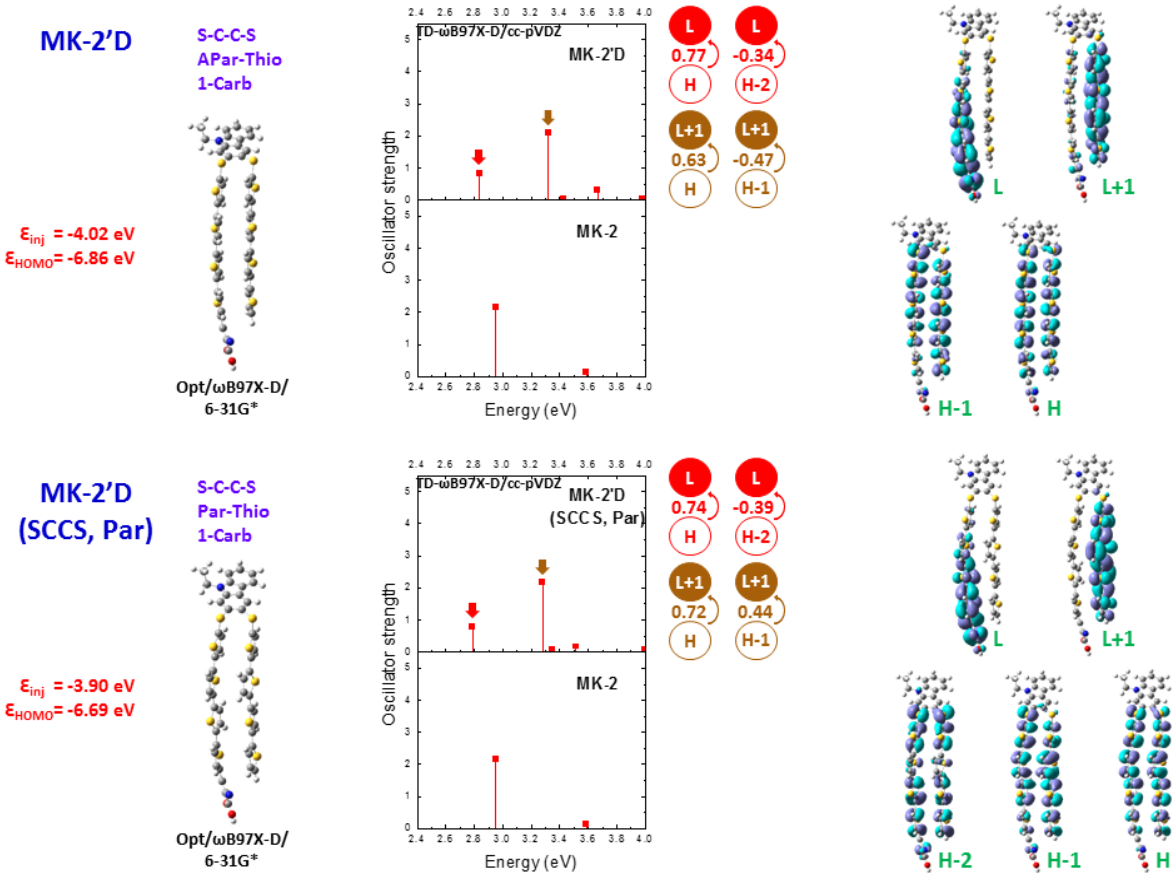
## 8. Properties of MK-3 and MK-2 and various designed dyes

### 8.1 MK-3 and MK-2



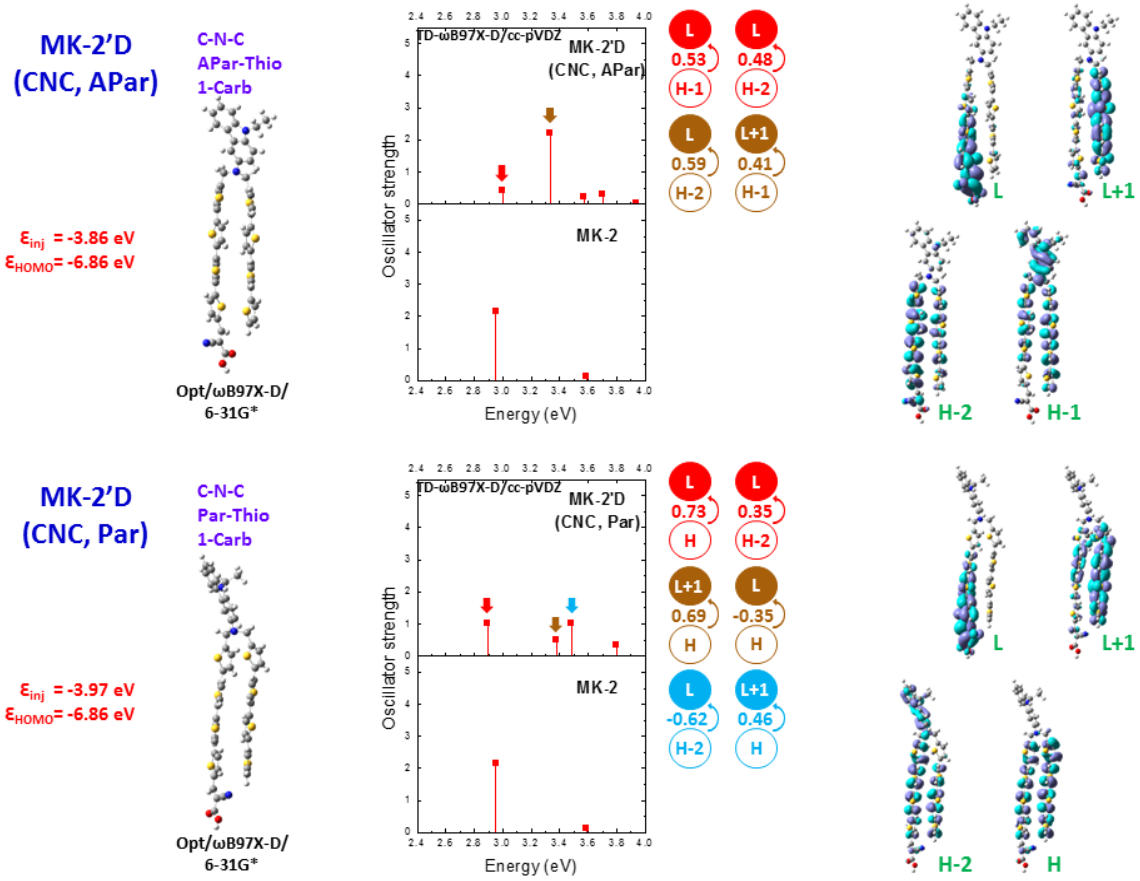

$\varepsilon_{inj}$ is defined as $\varepsilon_{HOMO} + \varepsilon_{S1}$, namely, the HOMO energy plus the first singlet excitation energy. $\varepsilon_{inj}$ is used as an estimate of ESOP, whereas $\varepsilon_{HOMO}$ is an estimate of GSOP. As can be seen, the LUMOs of both MK-3 and MK-2 are located largely on the anchoring group (acceptor), whereas their HOMOs, which do not extend to the acceptor, are spread over the π-bridges.

## 8.2 Dimeric dyes formed using S-C-C-S as the linker



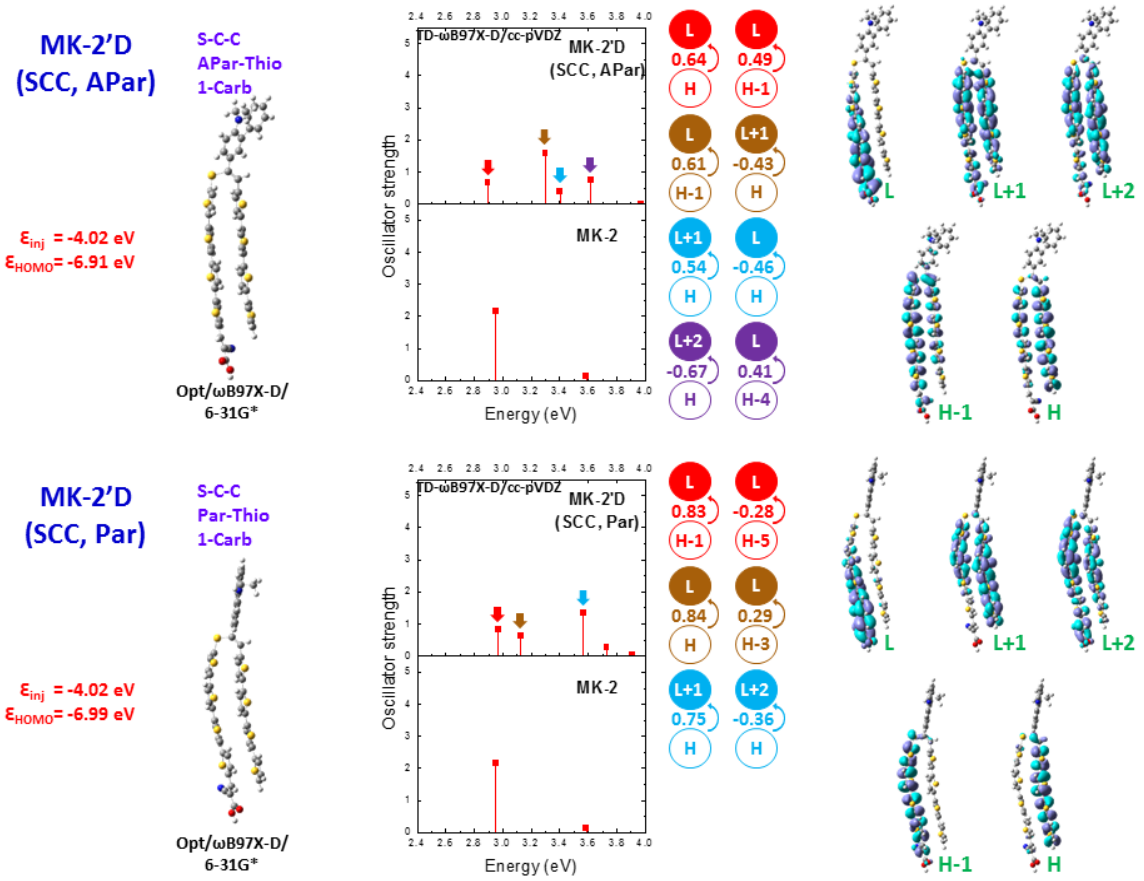

APar-Thio and Par-Thio stand for anti-parallel and parallel orientations of the two π-conjugated moieties, respectively. Compared to the anti-parallel orientation (upper panel, which corresponds to Fig. 2 of the main text), the parallel orientation renders both shallower $\varepsilon_{HOMO}$ and $\varepsilon_{inj}$. Both orientations result in a multi-peaked absorption.

### 8.3 Dimeric dyes formed using C-N-C as the linker



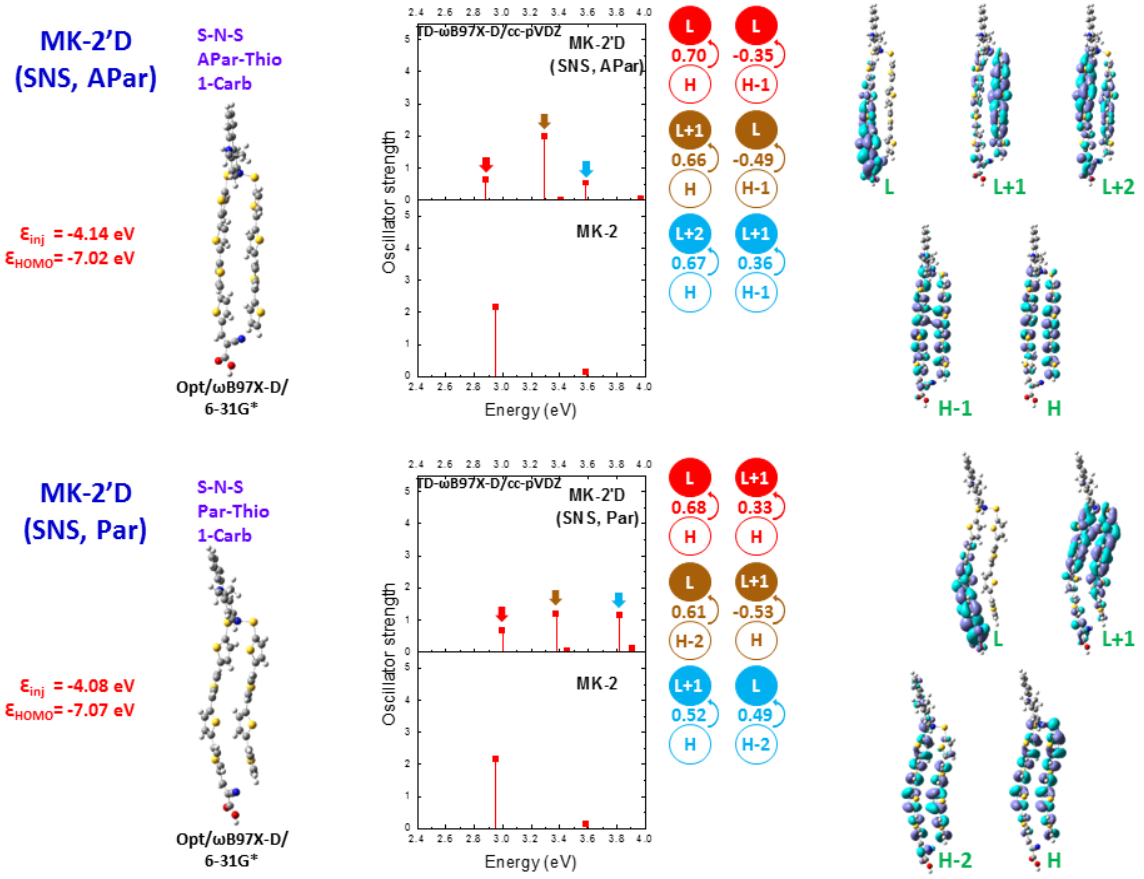

The parallel orientation renders an equal $\varepsilon_{HOMO}$ and a deeper $\varepsilon_{inj}$ compared to those of the anti-parallel orientation. Both orientations result in a multi-peaked absorption. The lowest absorption peak of the former, however, is lower in energy.

## 8.4 Dimeric dyes formed using S-C-C as the linker



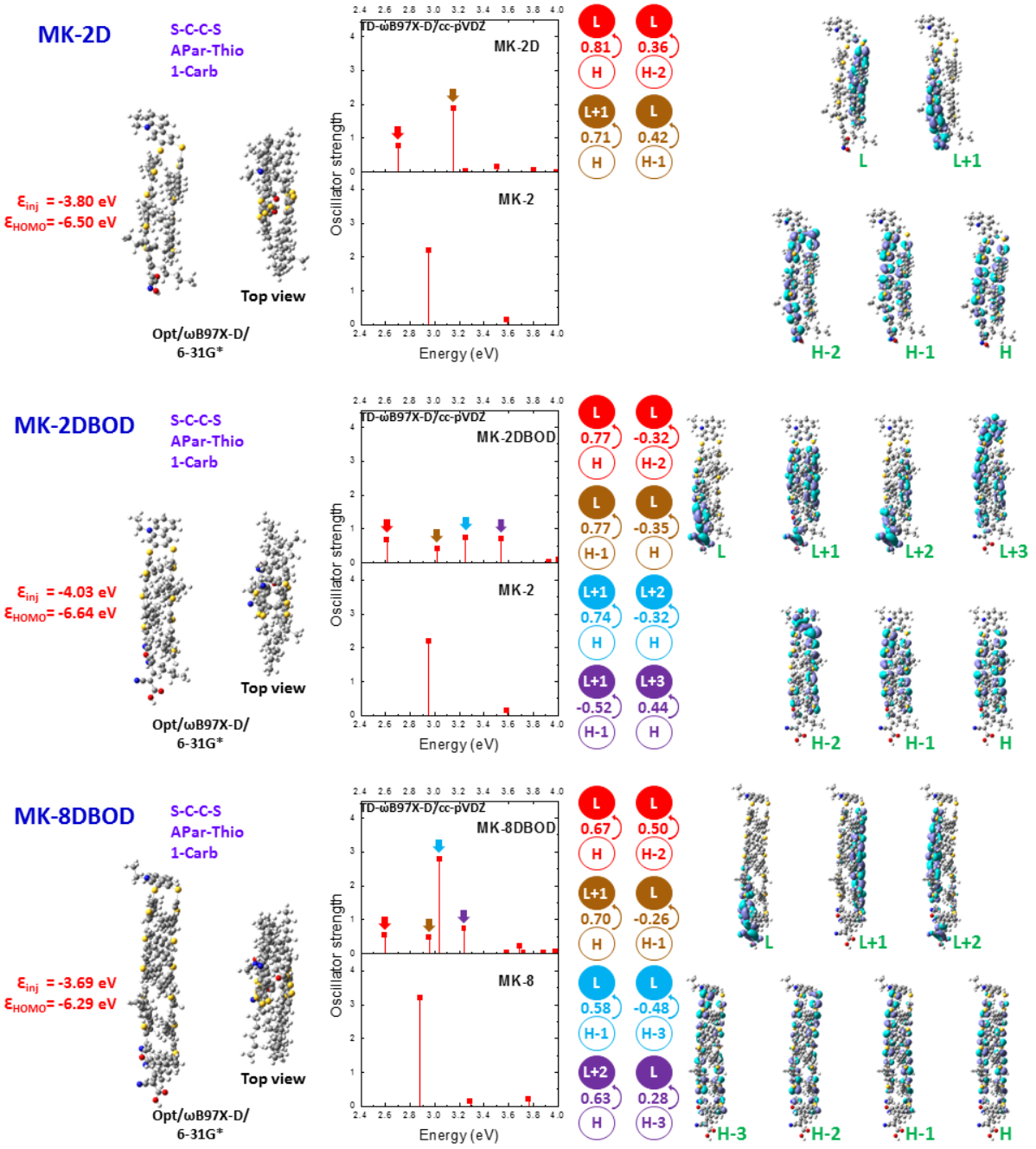

The parallel orientation renders a deeper $\varepsilon_{HOMO}$ and an equal $\varepsilon_{inj}$ compared to those of the anti-parallel orientation. Both orientations result in a multi-peaked absorption. The lowest absorption peak of the former is higher in energy.

## 8.5 Dimeric dyes formed using S-N-S as the linker



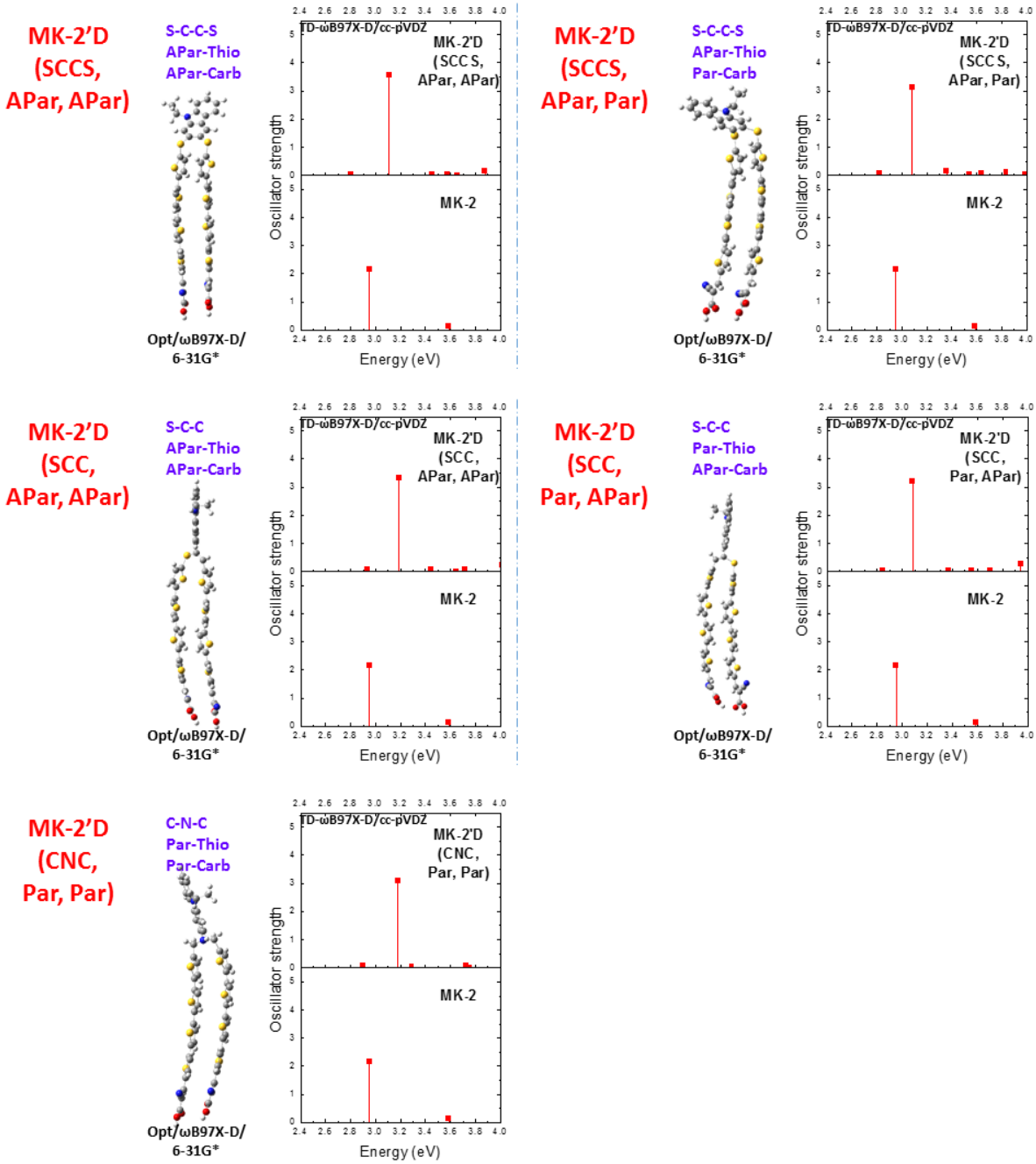

The parallel orientation renders a deeper $\varepsilon_{HOMO}$ and yet a shallower $\varepsilon_{inj}$ compared to those of the anti-parallel orientation. Both orientations result in a multi-peaked absorption. The lowest absorption peak of the former is higher in energy.

## 8.6 MK-2D, MK-2DBOD, and MK-8DBOD



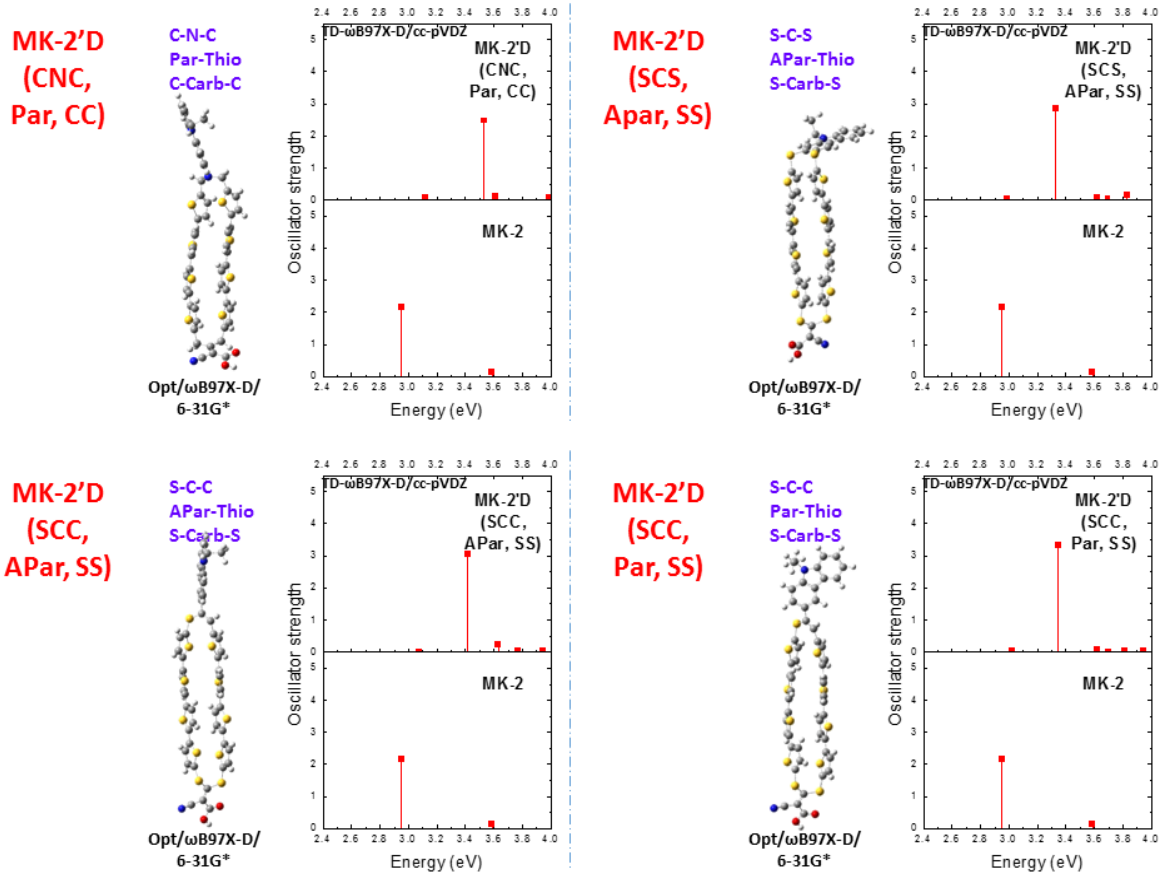

MK-2D has the same linker (S-C-C-S) and the same orientation (anti-parallel) as the MK-2'D but with the hexyl chains substituted to the dye. MK-2DBOD is formed by replacing the thiophene unit next to the cyanoacrylic acid with the BOD group. MK-8DBOD is formed by inserting one more thiophene unit to each π-conjugated oligomer of MK-2DBOD. Their absorption spectra compared to that of MK-2'D are plotted in Fig. 3 of the main text.

## 8.7 Dimeric dyes containing two cyanoacrylic acid anchoring groups




Independent of which linker is used and how the π-conjugated moieties or how the cyanoacrylic acid anchoring groups are oriented, all the dyes have an undesirable feature of single-peaked and blue-shifted absorption compared to the MK-2 dye due to distortions of the π-conjugated oligomers.

## 8.8 Dimeric dyes in which the two π-conjugated oligomers form a closed-loop




All the constructed dyes have an undesirable feature of single-peaked and blue-shifted absorption compared to the MK-2 dye due to distortions of the π-conjugated moieties.

## 9. Oxidation potentials of dyes

We examine the GSOP and ESOP, estimated respectively by $\varepsilon_{HOMO}$ and $\varepsilon_{inj}=\varepsilon_{HOMO}+\varepsilon_{S1}$, of several constructed dyes that respectively determine the efficiency of dye regeneration and electron injection in the associated DSSCs. According to our TD-ωB97X-D/cc-pVDZ results of WS-52 and WS-55[23] computed at the ωB97X-D/6-31G* optimized geometries (in vacuum), we set $\varepsilon_{HOMO}\leq$-6.64 eV (lower dash line) and $\varepsilon_{inj}\geq$-4.11 eV (upper dash line) as thresholds at the same computation level for an efficient dye regeneration and electron injection, respectively. Note that different environmental settings, e.g. redox mediators[24,25], solvents[26], and/or additives[27] of the DSSCs would change these thresholds.

Note that the absolute values of the computed oxidation potentials should not be directly compared with experiments, as that requires a detailed modelling of the dye environment and a precise computation of the oxidation potentials. It can be seen that the absolute values are too negative compared to experiment. However, their relative trends can be reasonably predicted by our computations. For example, the observed[23] (computed) HOMO energy difference between WS-52 and WS-55 is 0.15 V (0.19 V). Similarly, the observed (computed) LUMO level difference is 0.40 V (0.50 V). The computation results can be a useful reference when implementing these dyes in DSSCs.

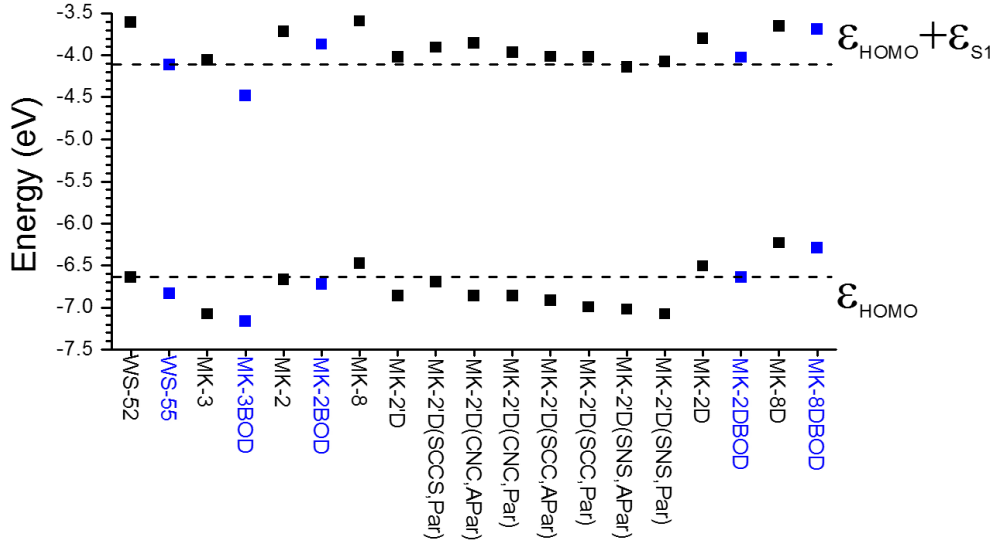



**Fig. S11** Energy levels of GSOP (estimated by $\varepsilon_{HOMO}$) and ESOP (estimated by $\varepsilon_{inj}$) of the known dyes (WS-52, WS-55, MK-3, MK-2, and MK-8) and several newly designed dyes computed by TD-ωB97X-D/cc-pVDZ at the ωB97X-D/6-31G* optimized geometries. Blue font colour denotes the dyes featuring the auxiliary BOD group.

## 10. References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# 11. Molecular coordinates of MK-2, MK-2'D, MK-2'D(CNC, Par, Par), MK-2D, MK-2DBOD, and MK-8DBOD at the ωB97X-D/6-31G* optimized geometries

## MK-2

| | | | |
|---|---|---|---|
| C | 12.8842384531 | -1.4185746959 | -0.2293181941 |
| C | 13.7911672793 | -0.3489640591 | -0.2450927511 |
| C | 13.3553171139 | 0.9692439635 | -0.2310152104 |
| C | 11.9789176194 | 1.1970308972 | -0.2032843786 |
| C | 11.0545538493 | 0.1299318150 | -0.1789809026 |
| C | 11.5169763265 | -1.1859525096 | -0.1950729642 |
| H | 13.2603917281 | -2.4364970301 | -0.2386455113 |
| H | 14.8574208354 | -0.5535691091 | -0.2649970027 |
| H | 14.0708184652 | 1.7857822174 | -0.2351966957 |
| H | 10.8126645912 | -2.0130252464 | -0.1764080458 |
| C | 9.9331511071 | 2.1240939812 | -0.1211507967 |
| C | 8.8539866468 | 3.0049240879 | -0.0488211970 |
| C | 7.5805756434 | 2.4644522691 | 0.0243613597 |
| C | 7.3559488866 | 1.0722659581 | 0.0149422101 |
| C | 8.4485124225 | 0.2067708511 | -0.0737931312 |
| C | 9.7375088998 | 0.7261375344 | -0.1232992787 |
| H | 8.9917533946 | 4.0814291727 | -0.0329013679 |
| H | 8.2950249230 | -0.8677268789 | -0.1112138397 |
| C | -10.7771776340 | 0.2655622113 | -1.2179155509 |
| N | -10.8738961697 | 1.2052749153 | -1.8911715838 |
| C | -11.8548215669 | -1.7447225945 | -0.1839461856 |
| C | -9.4547701886 | -1.4046071540 | 0.0157541741 |
| O | -12.9613457818 | -1.1899195237 | -0.6997811977 |
| H | -13.6926306873 | -1.7948713501 | -0.4994152090 |
| O | -11.8567218791 | -2.7999655165 | 0.4080676147 |
| C | 11.9389408626 | 4.2585202326 | 1.3040385355 |
| C | -4.2169637642 | -0.8129280739 | -0.3005086882 |
| C | -3.4860290029 | -1.9337690229 | -0.6494617632 |
| C | -2.0939780721 | -1.6566470602 | -0.7034633645 |
| C | -1.7490939021 | -0.3636516815 | -0.3948565735 |
| S | -3.1730603468 | 0.5545859210 | -0.0188344155 |
| H | -1.3527458731 | -2.3961863404 | -0.9815027672 |
| C | -10.6416405904 | -0.9179512615 | -0.4295849024 |
| C | 2.0862839413 | 0.3655175222 | -0.0752103747 |
| C | 1.4572077052 | 1.5643772854 | -0.3111567095 |
| C | 0.0465272302 | 1.4818163747 | -0.4557711177 |
| C | -0.4065370496 | 0.1858977264 | -0.3210200269 |
| S | 0.9082509606 | -0.9110727731 | -0.0081524961 |
| H | 1.9971952067 | 2.5018471189 | -0.3759867808 |
| C | 3.5144475700 | 0.1448244210 | 0.0807619349 |
| C | 4.2099915597 | -0.9352274668 | 0.5862592392 |
| C | 5.6145181579 | -0.6948885463 | 0.6043471055 |
| C | 5.9966806856 | 0.5256949824 | 0.1175107503 |
| S | 4.6050221030 | 1.4175889324 | -0.4030184436 |
| H | 6.3315254119 | -1.4022256934 | 1.0031327791 |
| N | 11.2860243902 | 2.3982699868 | -0.1937634274 |
| H | 6.7341326460 | 3.1389449259 | 0.1184072509 |
| C | 11.8624011049 | 3.7239880985 | -0.1245320846 |
| H | 12.8568044939 | 3.6861347088 | -0.5774369252 |
| H | 11.2573852052 | 4.3860639176 | -0.7532383291 |
| H | 12.3530501558 | 5.2715257504 | 1.3127644752 |
| H | 10.9428034798 | 4.2883947313 | 1.7555754457 |
| H | 12.5732698613 | 3.6164213088 | 1.9218243051 |
| C | 3.5815402330 | -2.2175599703 | 1.0787009966 |
| H | 2.8172850725 | -1.9868701090 | 1.8335144137 |
| H | 3.0459096183 | -2.6969128905 | 0.2469207314 |
| C | 4.5703392381 | -3.2316154477 | 1.6553942991 |
| H | 5.3314963527 | -3.4697288646 | 0.9008078282 |
| H | 5.0987570423 | -2.7860561365 | 2.5088723351 |
| C | 3.8985470906 | -4.5288656084 | 2.1028055792 |
| H | 3.1403127111 | -4.3086724967 | 2.8668137631 |
| H | 3.3625446440 | -4.9730956936 | 1.2519860199 |
| C | 4.9013192281 | -5.5435852357 | 2.6520713783 |

| | | | |
|---|---|---|---|
| H | 5.6675990090 | -5.7448567139 | 1.8899463202 |
| H | 5.4286368691 | -5.1012266093 | 3.5094732450 |
| C | 4.2636931447 | -6.8648742458 | 3.0814543149 |
| H | 3.5002365689 | -6.6681274799 | 3.8455405875 |
| H | 3.7380023297 | -7.3060539933 | 2.2239014220 |
| C | 5.2882814959 | -7.8619158349 | 3.6204076971 |
| H | 5.8019669151 | -7.4532906289 | 4.4984924382 |
| H | 4.8173937624 | -8.8042137753 | 3.9189706504 |
| H | 6.0488659773 | -8.0898162627 | 2.8649876449 |
| C | -0.8387013153 | 2.6703729861 | -0.7391732146 |
| H | -1.5539152235 | 2.3995587842 | -1.5273872018 |
| H | -1.4498836205 | 2.8930505947 | 0.1469634490 |
| C | -0.1095696010 | 3.9503337228 | -1.1523056145 |
| H | 0.4847166364 | 4.3286663231 | -0.3095549061 |
| H | 0.5978858697 | 3.7327975614 | -1.9630840048 |
| C | -1.0876737485 | 5.0325202819 | -1.6097496451 |
| H | -1.6329339479 | 4.6708075033 | -2.4930154238 |
| H | -1.8422537511 | 5.1997788169 | -0.8282818003 |
| C | -0.4054259214 | 6.3587220089 | -1.9432531092 |
| H | 0.1097476138 | 6.7383203725 | -1.0492706538 |
| H | 0.3722293996 | 6.1886157629 | -2.7010939717 |
| C | -1.3816980896 | 7.4220344712 | -2.4497191387 |
| H | -2.1681187685 | 7.5778726159 | -1.6995488213 |
| H | -1.8820176244 | 7.0481542969 | -3.3528688464 |
| C | -0.6948029170 | 8.7519858201 | -2.7557897594 |
| H | 0.0801064712 | 8.6251076585 | -3.5203991322 |
| H | -1.4100765041 | 9.4970103711 | -3.1193967062 |
| H | -0.2157721102 | 9.1605705770 | -1.8584633372 |
| C | -4.0731126214 | -3.2880460336 | -0.9647445377 |
| H | -4.5717001283 | -3.6837672595 | -0.0683875514 |
| H | -4.8601479949 | -3.1735158611 | -1.7222273544 |
| C | -3.0641188275 | -4.3275643949 | -1.4562515803 |
| H | -2.5598518930 | -3.9494384466 | -2.3554325730 |
| H | -2.2876195873 | -4.4807829382 | -0.6955101043 |
| C | -3.7212040887 | -5.6704180561 | -1.7727750507 |
| H | -4.2226309378 | -6.0535485546 | -0.8728530017 |
| H | -4.5052837642 | -5.5248607445 | -2.5285666302 |
| C | -2.7179581064 | -6.7100369426 | -2.2730005569 |
| H | -2.2191887149 | -6.3243411707 | -3.1736221938 |
| H | -1.9307962320 | -6.8486342314 | -1.5183725770 |
| C | -3.3550217413 | -8.0632237806 | -2.5900061246 |
| H | -3.8488734859 | -8.4508176199 | -1.6889238611 |
| H | -4.1432006474 | -7.9239371809 | -3.3415319434 |
| C | -2.3380213758 | -9.0862874858 | -3.0940801423 |
| H | -1.8541635143 | -8.7332720235 | -4.0120426148 |
| H | -1.5544702797 | -9.2599397513 | -2.3477579397 |
| H | -2.8113509035 | -10.0489867731 | -3.3132049640 |
| C | -5.6485195368 | -0.6168733827 | -0.1663683711 |
| C | -6.3002337662 | 0.5847168376 | 0.0143861797 |
| C | -7.7103495044 | 0.4959348580 | 0.1004508837 |
| C | -8.1456149346 | -0.8151933313 | -0.0309259118 |
| S | -6.7990227204 | -1.9127541274 | -0.2056118214 |
| H | -5.7733335998 | 1.5291142080 | 0.0849609696 |
| C | -8.5909474051 | 1.6771443969 | 0.4026474757 |
| H | -8.8612185908 | 2.1829045966 | -0.5331491247 |
| H | -9.5370203888 | 1.3133173941 | 0.8187036143 |
| C | -7.9881919891 | 2.6922880375 | 1.3794321890 |
| H | -7.1088819495 | 3.1740494898 | 0.9316583721 |
| H | -7.6327735950 | 2.1759288004 | 2.2810297789 |
| C | -9.0038025730 | 3.7652535471 | 1.7686433733 |
| H | -9.3725992198 | 4.2602039726 | 0.8594181833 |
| H | -9.8801389079 | 3.2841167502 | 2.2257100870 |
| C | -8.4470236374 | 4.8126296011 | 2.7310571533 |
| H | -7.5777623158 | 5.3049310109 | 2.2714892205 |
| H | -8.0699886274 | 4.3162790080 | 3.6368618867 |
| C | -9.4772372077 | 5.8697576142 | 3.1276302984 |
| H | -9.8537622943 | 6.3615645891 | 2.2207261415 |
| H | -10.3446326251 | 5.3762725689 | 3.5863527481 |
| C | -8.9214574557 | 6.9192676580 | 4.0877063034 |
| H | -8.0652708041 | 7.4400740098 | 3.6429304817 |
| H | -9.6770437003 | 7.6699135399 | 4.3404084799 |

| | | | |
|---|---|---|---|
| H | -8.5771125453 | 6.4598362392 | 5.0214482547 |
| H | -9.5217176528 | -2.4041708669 | 0.4443975188 |

## MK-2’D

| | | | |
|---|---|---|---|
| C | -11.0297855985 | 4.2607565346 | -0.9686724168 |
| C | -11.4056441379 | 3.8280388660 | -2.2497615006 |
| C | -10.9748531819 | 2.6114404935 | -2.7588632190 |
| C | -10.1538259885 | 1.8236630691 | -1.9505272076 |
| C | -9.7792143896 | 2.2401436938 | -0.6549480004 |
| C | -10.2200935927 | 3.4712304194 | -0.1667204915 |
| H | -11.3850164320 | 5.2182496110 | -0.6014450736 |
| H | -12.0460812430 | 4.4577550125 | -2.8592363478 |
| H | -11.2844265368 | 2.2846586343 | -3.7465543347 |
| H | -9.9287728145 | 3.8057670035 | 0.8251256637 |
| C | -8.8846458999 | 0.1819448153 | -1.1004438959 |
| C | -8.1768068670 | -0.9990658407 | -0.8796500636 |
| C | -7.5485899122 | -1.1856659241 | 0.3486434864 |
| C | -7.6130589577 | -0.1888349011 | 1.3565954492 |
| C | -8.3202222912 | 0.9862854286 | 1.1113224996 |
| C | -8.9646042224 | 1.1792394733 | -0.1071499195 |
| H | -8.1039283562 | -1.7724203936 | -1.6372383563 |
| H | -8.3711341325 | 1.7455767590 | 1.8853652096 |
| C | 11.6755022180 | -0.8771096613 | 0.0112305121 |
| N | 11.9070872688 | -1.6763970644 | 0.8200281587 |
| C | 12.3715581394 | 1.0609607852 | -1.4282804373 |
| C | 10.1026566521 | 0.2020721674 | -1.5310216703 |
| O | 13.5556690695 | 0.8569273274 | -0.8326391713 |
| H | 14.1609085412 | 1.5281575733 | -1.1848993461 |
| O | 12.1782161368 | 1.9441373314 | -2.2337020942 |
| C | -10.9175450876 | -1.2027173526 | -3.3011936348 |
| C | 5.0487816724 | -1.1363348865 | -1.3237833958 |
| C | 4.2747403708 | -0.1102363958 | -1.8039047326 |
| C | 2.8877956042 | -0.3360832414 | -1.6559852058 |
| C | 2.5958740587 | -1.5366630015 | -1.0576171497 |
| S | 4.0509696765 | -2.4256843376 | -0.7160515294 |
| H | 2.1303946079 | 0.3934272797 | -1.9185127258 |
| C | 11.3399333260 | 0.0926805981 | -0.9794305565 |
| C | -1.1750199203 | -2.3241310980 | -0.3721256767 |
| C | -0.4324691162 | -3.1666350706 | 0.4161376320 |
| C | 0.9665315360 | -3.0035724805 | 0.2466936508 |
| C | 1.2928824709 | -2.0374129843 | -0.6711220141 |
| S | -0.1419272952 | -1.3431692728 | -1.3666463826 |
| H | -0.8767096697 | -3.8538440363 | 1.1277466744 |
| C | -2.6098434623 | -2.1249615134 | -0.4122624398 |
| C | -3.2840361242 | -1.0048220066 | -0.8124401022 |
| C | -4.6862833891 | -1.0726114045 | -0.5961393981 |
| C | -5.0724840855 | -2.2456831565 | -0.0142181306 |
| S | -3.7212929442 | -3.3157120438 | 0.2157261451 |
| H | -5.3723545105 | -0.2643222088 | -0.8131364493 |
| N | -9.5826229343 | 0.5879444030 | -2.2176427129 |
| C | -9.7761713802 | -0.1960105333 | -3.4204897509 |
| H | -9.9579872886 | 0.5015987597 | -4.2427667652 |
| H | -8.8334973022 | -0.7045016447 | -3.6500819781 |
| H | -11.0439568134 | -1.7454768938 | -4.2432333319 |
| H | -10.7132330449 | -1.9301536711 | -2.5095844097 |
| H | -11.8572838808 | -0.6942625168 | -3.0642479840 |
| C | 6.4890477038 | -1.1531276134 | -1.1908016160 |
| C | 7.2762135188 | -1.9353446893 | -0.3665172222 |
| C | 8.6393571081 | -1.5888038023 | -0.4061735388 |
| C | 8.9087831426 | -0.5411072910 | -1.2683928995 |
| S | 7.4484470283 | -0.0158709438 | -2.0591332369 |
| H | 6.8728560082 | -2.7063315553 | 0.2801564457 |
| H | 10.0214479267 | 1.0037237085 | -2.2634452587 |
| C | 4.7491492557 | 1.5398552176 | 1.1237451103 |
| C | 4.4917896593 | 0.3310177725 | 1.7150915394 |
| C | 3.1094210941 | 0.0831366793 | 1.9075586176 |
| C | 2.3053656658 | 1.1016857147 | 1.4665767507 |
| S | 3.2674698499 | 2.4101668739 | 0.8377668516 |
| H | 2.7166534465 | -0.8432248039 | 2.3114275415 |
| C | -1.5757327427 | 0.7380874972 | 1.8866671945 |

| | | | |
|---|---|---|---|
| C | -1.3526518628 | 1.7184079738 | 0.9535442348 |
| C | 0.0254837282 | 1.9573317420 | 0.7091418095 |
| C | 0.8558108047 | 1.1608127867 | 1.4573874922 |
| S | -0.0704194719 | 0.1200774253 | 2.4946241721 |
| H | -2.1557614608 | 2.2337520999 | 0.4378491709 |
| C | -2.8281646131 | 0.1751515336 | 2.3602818984 |
| C | -3.0169710829 | -1.0703525408 | 2.9011922731 |
| C | -4.3790239736 | -1.3715096107 | 3.1550646291 |
| C | -5.2249810883 | -0.3542441342 | 2.8172935875 |
| S | -4.3406935358 | 1.0250742640 | 2.2227705485 |
| H | -4.7355119749 | -2.3238115254 | 3.5283068653 |
| C | 6.0319027755 | 2.0911988289 | 0.7200358690 |
| C | 6.2979030995 | 3.0489714900 | -0.2261210022 |
| C | 7.6870207154 | 3.3262588117 | -0.3683276321 |
| C | 8.4604905112 | 2.5757612010 | 0.4671025204 |
| S | 7.5065624590 | 1.5339732527 | 1.4532681618 |
| H | 5.5239759925 | 3.5299794330 | -0.8145595108 |
| H | 9.3943172306 | -2.0747532959 | 0.1984511614 |
| H | 8.0896005418 | 4.0440957173 | -1.0732188775 |
| H | 4.6913782232 | 0.8148662364 | -2.1862955486 |
| H | 0.3881076843 | 2.6784620716 | -0.0153076261 |
| H | 1.7048058546 | -3.5593454169 | 0.8141493672 |
| H | -2.7870172746 | -0.1221235982 | -1.1993040445 |
| H | -2.2106120699 | -1.7802251046 | 3.0471192083 |
| H | 5.2689770293 | -0.3850215244 | 1.9576677925 |
| S | -6.9726970241 | -0.3714445177 | 3.0206225334 |
| S | -6.6721925791 | -2.7308261117 | 0.5670249163 |
| H | 9.5381917431 | 2.5724811235 | 0.5548221305 |

## MK-2'D(CNC, Par, Par)

| | | | |
|---|---|---|---|
| C | -14.3705035580 | 1.7073505415 | 1.8018092694 |
| C | -14.9891339787 | 2.3091818552 | 0.6962126966 |
| C | -14.3132257493 | 2.4904408748 | -0.5024420868 |
| C | -12.9891122141 | 2.0561043255 | -0.5697367924 |
| C | -12.3535311293 | 1.4409290914 | 0.5318046412 |
| C | -13.0556125177 | 1.2694085655 | 1.7259581622 |
| H | -14.9274569820 | 1.5817045441 | 2.7252466241 |
| H | -16.0189010137 | 2.6451002131 | 0.7741217366 |
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| H | -12.5805525075 | 0.8019964150 | 2.5840631588 |
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