Electronic Supplementary Information for:

# Two-Step Model for Ultrafast Interfacial Electron Transfer: Limitations of Fermi's Golden Rule Revealed by Quantum Dynamics Simulations

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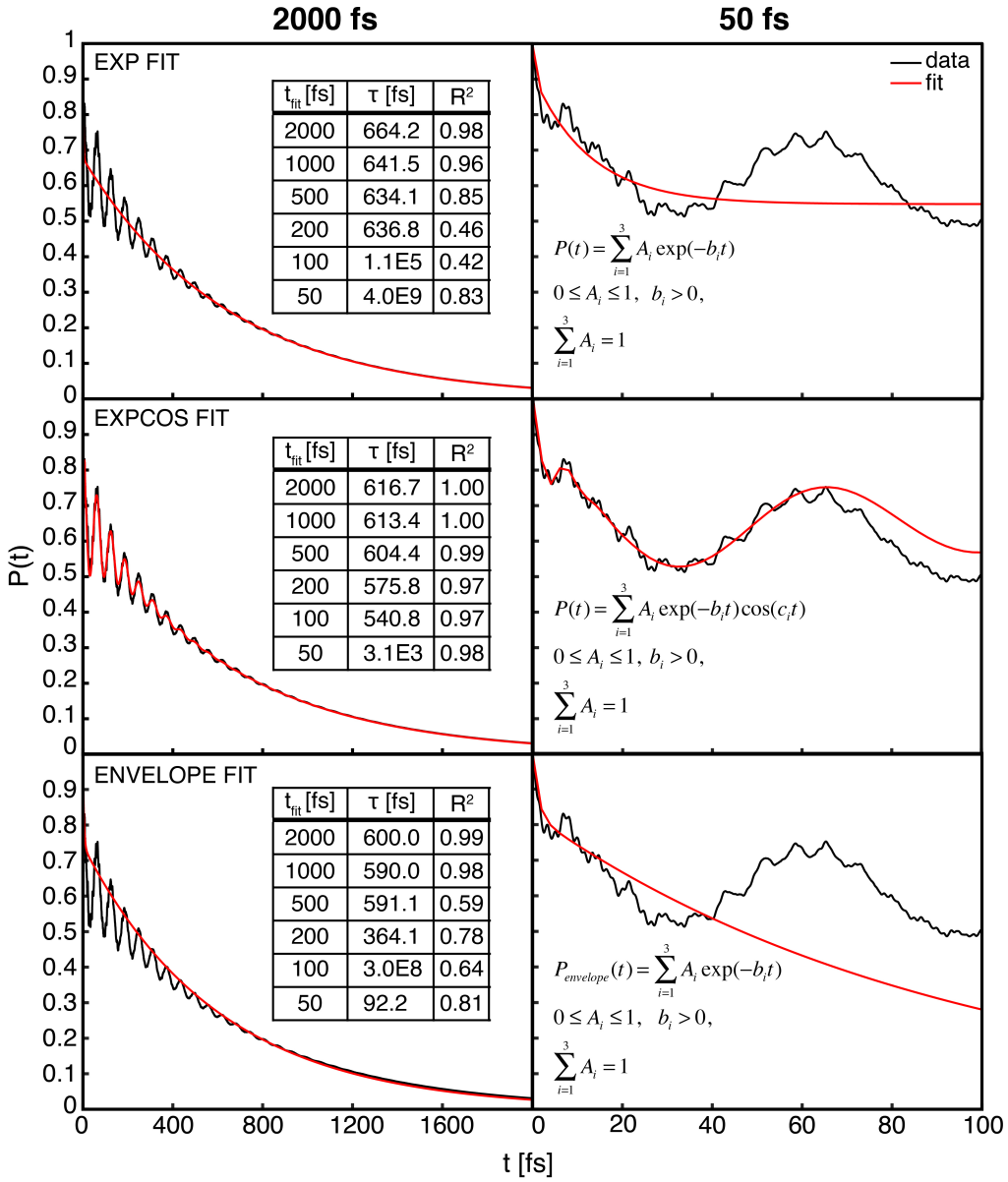
## 1. Method comparison for fitting the characteristic IET time




| $t_{fit}$ [fs] | τ [fs] | $R^2$ |
|---|---|---|
| 2000 | 664.2 | 0.98 |
| 1000 | 641.5 | 0.96 |
| 500 | 634.1 | 0.85 |
| 200 | 636.8 | 0.46 |
| 100 | 1.1E5 | 0.42 |
| 50 | 4.0E9 | 0.83 |

| $t_{fit}$ [fs] | τ [fs] | $R^2$ |
|---|---|---|
| 2000 | 616.7 | 1.00 |
| 1000 | 613.4 | 1.00 |
| 500 | 604.4 | 0.99 |
| 200 | 575.8 | 0.97 |
| 100 | 540.8 | 0.97 |
| 50 | 3.1E3 | 0.98 |

| $t_{fit}$ [fs] | τ [fs] | $R^2$ |
|---|---|---|
| 2000 | 600.0 | 0.99 |
| 1000 | 590.0 | 0.98 |
| 500 | 591.1 | 0.59 |
| 200 | 364.1 | 0.78 |
| 100 | 3.0E8 | 0.64 |
| 50 | 92.2 | 0.81 |

**Figure S1.** Comparison of different fitting methods with 2 ps and 50 fs fitting times. Black lines represent survival probabilities for simulations with LUMO initial state on one of the MD sampled bidentate structures. Characteristic IET times and corresponding $R^2$ for the fits are listed in the tables on the left.

For consistency, all overall characteristic times were fitted with 3 exponential components. Three different fitting schemes were tested. The exponential fitting utilizes a sum of three exponential functions to fit the survival probability curve:

$$P(t)=\sum_{i=1}^{3} A_i \exp(-b_i t)$$

with the following constraints:

$$\sum_{i=1}^{3} A_i = 1,\ 0 \le A_i \le 1, \text{ and } b_i > 0$$

A representative exponential fit is shown in Figure S1 (top).

Since an exponential fit is not able to capture the rapid oscillations seen in the survival probability curve, a fitting scheme containing a periodic cos function was also tested:

$$P(t) = \sum_{i=1}^{3} A_i \exp(-b_i t)\cos(c_i t)$$

A representative fit for this functional form is shown in the second row of Figure S1. While this functional form successfully reproduces the oscillation of the survival probability curve, it contains 9 parameters and is non-linear, making the results very sensitive to the initial parameter guess.

When calculating the characteristic IET time, only the exponential parts, which correspond to the upper envelope of the curve, are used. Therefore, we also tested direct fitting of the curve envelope with tri-exponential functions. The envelope fitting approach uses the top 10% of data points (or at least 50 data points) for fitting, and results are shown in the bottom panel of Figure S1. The envelope fitting method, in principle, should give the same result as oscillation exponential decay function. However, in practice, envelope point selection decreases the number of data points used for fitting. Moreover, the points selected are not the true envelope points but its approximation, and the fitting results diverge from results obtained with oscillating exponential decay function.

Different fitting lengths from 50 fs to 2000 fs were also tested, and the results are listed in Figure S1. For fitting times longer than 500 fs, all three fitting methods give very similar results. The results start to diverge for shorter fitting times. This is true for all other IET curves. Since utilizing a simple exponential function leads to similar fitting results as two more sophisticated fitting methods (provided the time interval is long enough), we elected to use the simple 3-component exponential function for all subsequent fits.

## 2. Calculation of the number of the $TiO_2$ acceptor states

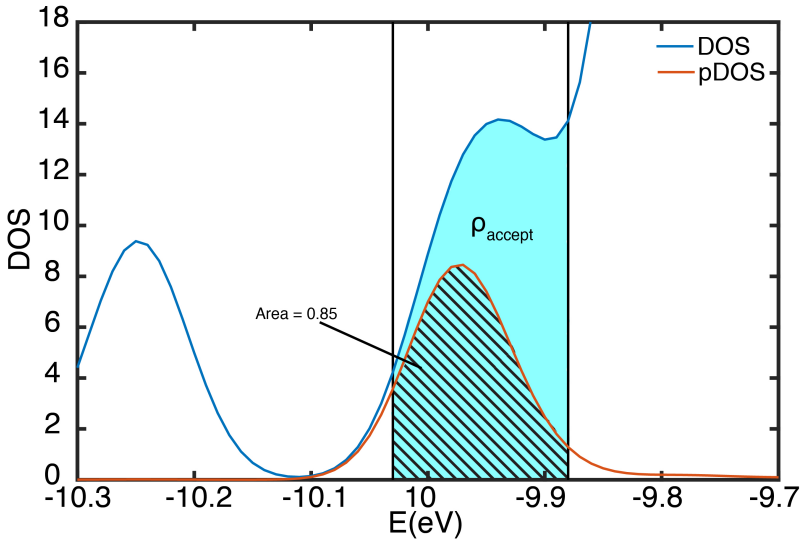



**Figure S2.** Example of a calculation of the number of $TiO_2$ acceptor states. Left and right boundaries are chosen so as to make the area of pDOS of the dye between two boundaries (patterned region) to be equal to 0.85. The number of acceptor states is equal to the area covered by DOS curve (cyan region).

## 3. $R^2$ values for correlations between the calculated IET characteristic times and selected electronic and structural parameters

**Table S1.** $R^2$ for linear fits between log(τ), overall characteristic time, and selected electronic and structural parameters. Values of $R^2$ larger than 0.1 are bolded.

| | Mono | | | Bi | | | Mono, Bi | | |
|---|---|---|---|---|---|---|---|---|---|
| | L | L+1 | L, L+1 | L | L+1 | L, L+1 | L | L+1 | L, L+1 |
| $E_{MO}$ | **0.17** | 0.06 | **0.17** | **0.36** | 0.02 | **0.35** | **0.14** | 0.04 | 0.05 |
| log(%$\rho_{linker}$) | 0.02 | 0.01 | **0.19** | 0.02 | **0.35** | 0.10 | 0.05 | **0.20** | 0.00 |
| log($\rho_{accept}$) | **0.37** | 0.05 | 0.00 | **0.24** | 0.05 | **0.38** | 0.08 | 0.07 | **0.11** |
| log($\rho_{accept}$+) | **0.18** | 0.05 | **0.15** | **0.40** | 0.03 | **0.42** | **0.11** | 0.04 | 0.06 |
| log($\rho_{surface}$) | **0.4** | **0.10** | 0.01 | **0.31** | 0.07 | **0.37** | 0.00 | **0.10** | 0.02 |
| log($\rho_{bulk}$) | **0.45** | 0.05 | 0.01 | **0.23** | 0.05 | **0.36** | **0.11** | 0.07 | **0.13** |
| R(O-Ti) | 0.01 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | **0.29** | 0.01 | 0.09 |

**Table S2.** $R^2$ for linear fits between log($\tau_{ini}$), initial characteristic time, and selected electronic and structural parameters. Values of $R^2$ larger than 0.1 are bolded.

| | Mono | | | Bi | | | Mono, Bi | | |
|---|---|---|---|---|---|---|---|---|---|
| | L | L+1 | L, L+1 | L | L+1 | L, L+1 | L | L+1 | L, L+1 |
| $E_{MO}$ | 0.06 | 0.00 | **0.59** | **0.41** | 0.02 | **0.42** | **0.17** | 0.01 | **0.49** |
| log(%$\rho_{linker}$) | 0.00 | **0.19** | **0.60** | 0.00 | **0.81** | **0.83** | 0.00 | **0.51** | **0.70** |
| log($\rho_{accept}$) | **0.53** | **0.15** | 0.05 | **0.68** | **0.23** | 0.02 | **0.55** | **0.17** | 0.03 |
| log($\rho_{accept}$+) | 0.07 | 0.01 | **0.57** | **0.34** | 0.02 | **0.37** | **0.17** | 0.01 | **0.44** |
| log($\rho_{surface}$) | **0.62** | **0.21** | 0.01 | **0.80** | **0.26** | 0.00 | **0.51** | **0.12** | 0.00 |
| log($\rho_{bulk}$) | **0.52** | **0.15** | 0.03 | **0.58** | **0.22** | 0.02 | **0.52** | **0.17** | 0.03 |
| R(O-Ti) | 0.08 | 0.02 | 0.02 | 0.04 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

## 4. Correlation plots for the selected parameters and characteristic IET times

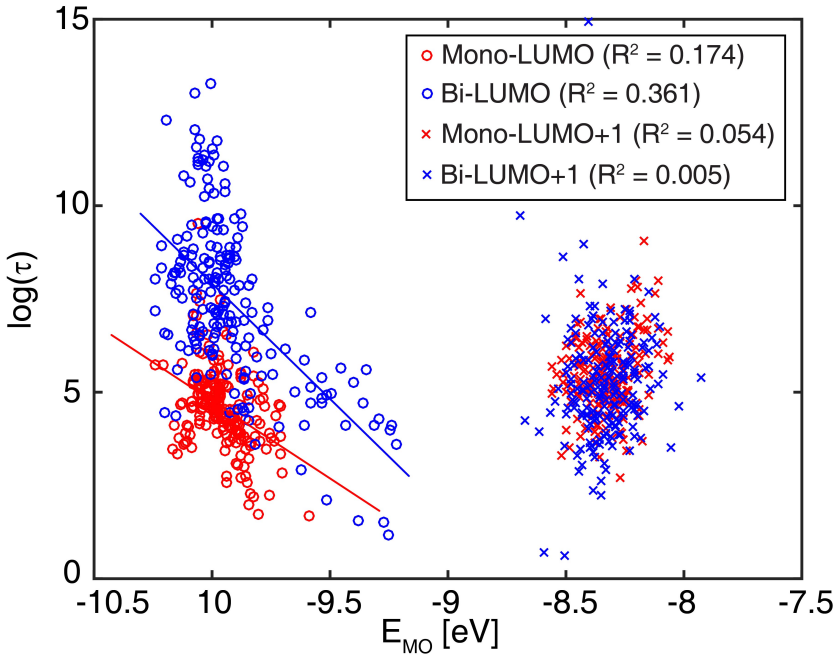



**Figure S3.** Correlation plots for the energy of particle state and log(τ). LUMO initial states are labeled as circles, while LUMO+1 initial states are represented as crosses. Mono and Bi are shown in red and blue, respectively. For the LUMO initial state, the trend lines are also drawn.

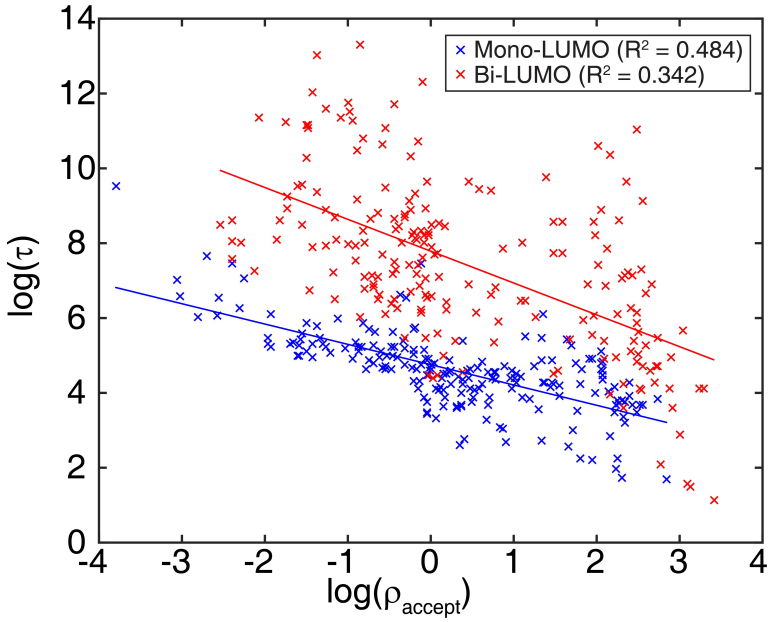



**Figure S4.** Correlation plots for the logarithm of the number of available acceptor states on $TiO_2$ slab for coupling with pyridine's LUMO particle state and log(τ).

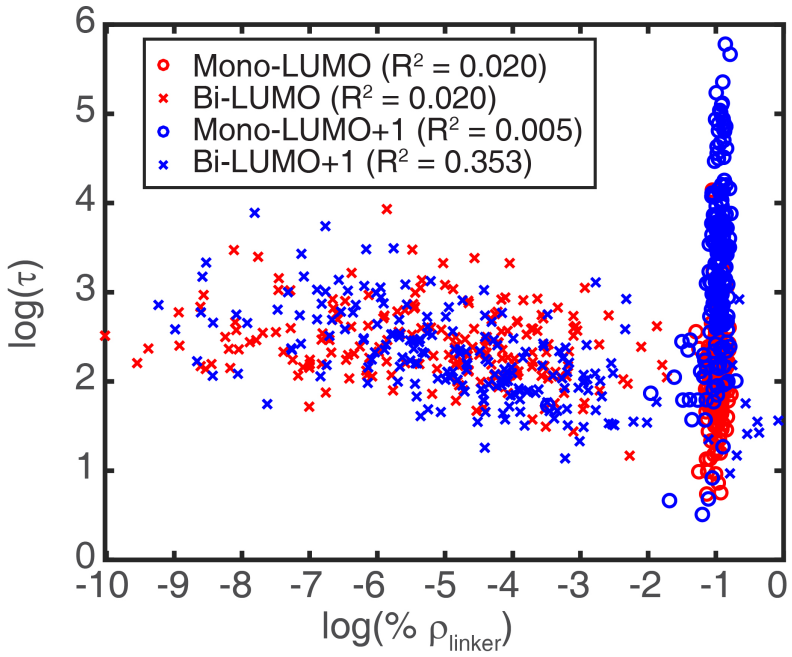



**Figure S5.** Correlation plots for the electron density on the linker group and log(τ).

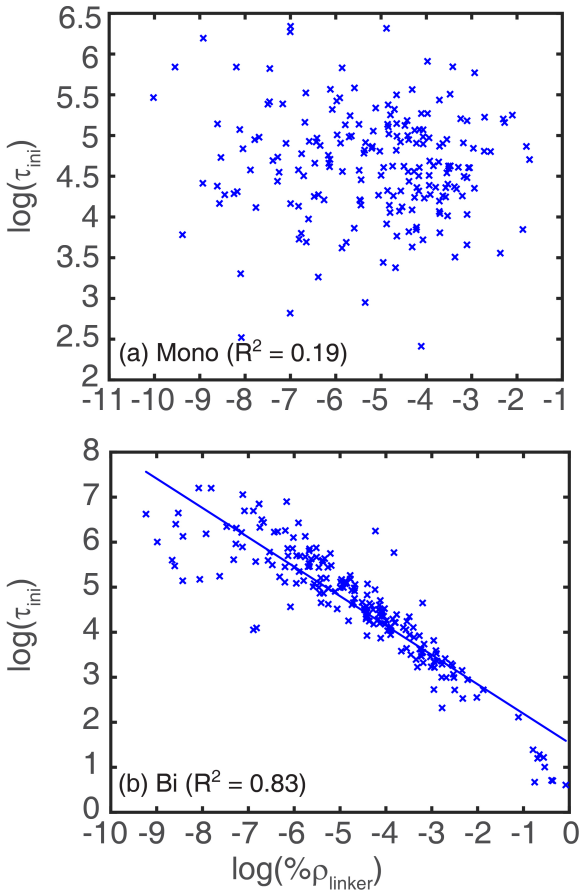



**Figure S6.** Correlation plots for the electron density on the linker group and log($\tau_{ini}$) for the LUMO+1 initial state.

## 5. Wavepacket survival probabilities in the surface region

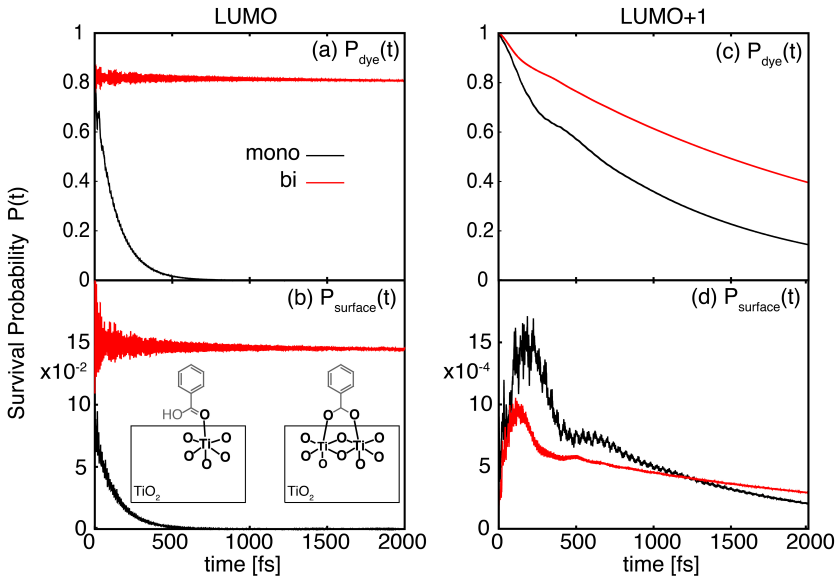



**Figure S7.** Survival probabilities on the first layer of $TiO_2$ slab connected to the dye. Surface regions are defined as a $TiO_8$ or $Ti_2O_{10}$ cluster for the monodentate and bidentate attachment modes, respectively (highlighted in black in schematic figures). Bulk regions are defined as the remainder of the $TiO_2$ slab.

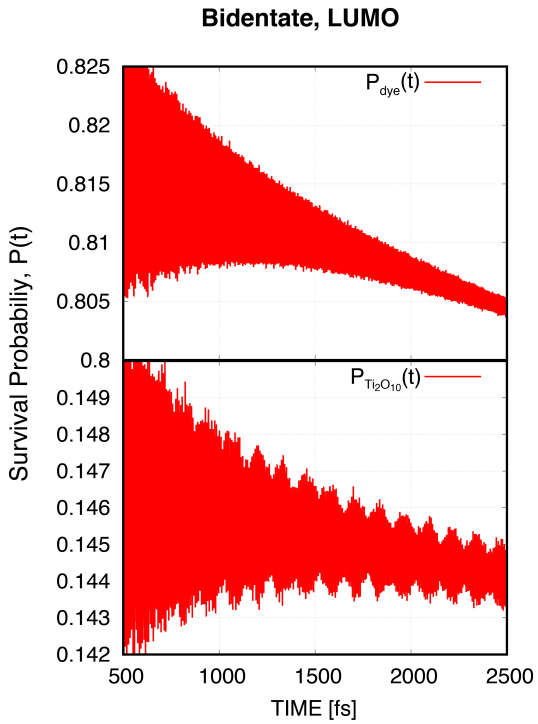



**Figure S8.** Survival probabilities on the dye and the first layer of $TiO_2$ slab for pyCA-$TiO_2$ in the bidentate attachment mode, showing injection from the LUMO initial state. The figure provides a closer look at medium-long term dynamics.

## 6. DFT-optimized coordinates for pyridine-$TiO_2$ slab

**Table S3.** XYZ coordinates for the monodentate attachment mode

| ATOM | X | Y | Z |
|---|---|---|---|
| H | 5.96863 | 3.69409 | 11.09198 |
| H | 5.48029 | 4.75460 | 14.36871 |
| H | 8.38201 | 7.38052 | 12.54687 |
| H | 5.85571 | 5.97854 | 16.52754 |
| H | 8.60862 | 8.52533 | 14.77172 |
| Ti | 0.00000 | 1.58260 | 1.10335 |
| Ti | 1.90594 | 6.82612 | 1.10336 |
| Ti | 1.90594 | 3.85797 | 1.99114 |
| Ti | 0.00000 | 9.10149 | 1.99114 |
| Ti | 0.00000 | 0.19704 | 4.65450 |
| Ti | 1.90594 | 5.44057 | 4.65450 |
| Ti | 1.90594 | 2.47241 | 5.54228 |
| Ti | 0.00000 | 7.71594 | 5.54229 |
| Ti | 15.24162 | 9.28125 | 8.34672 |
| Ti | 1.90644 | 4.03190 | 8.34312 |
| Ti | 1.90270 | 1.18887 | 9.01597 |
| Ti | 15.23825 | 6.42582 | 9.00844 |
| Ti | 3.81187 | 1.58260 | 1.10335 |
| Ti | 7.62375 | 1.58260 | 1.10335 |
| Ti | 11.43562 | 1.58260 | 1.10335 |
| Ti | 5.71781 | 6.82612 | 1.10336 |
| Ti | 9.52969 | 6.82612 | 1.10336 |
| Ti | 13.34156 | 6.82612 | 1.10336 |
| Ti | 5.71781 | 3.85797 | 1.99114 |
| Ti | 9.52969 | 3.85797 | 1.99114 |
| Ti | 13.34156 | 3.85797 | 1.99114 |
| Ti | 3.81187 | 9.10149 | 1.99114 |
| Ti | 7.62375 | 9.10149 | 1.99114 |
| Ti | 11.43562 | 9.10149 | 1.99114 |
| Ti | 3.81187 | 0.19704 | 4.65450 |
| Ti | 7.62375 | 0.19704 | 4.65450 |
| Ti | 11.43562 | 0.19704 | 4.65450 |
| Ti | 5.71781 | 5.44057 | 4.65450 |
| Ti | 9.52969 | 5.44057 | 4.65450 |
| Ti | 13.34156 | 5.44057 | 4.65450 |
| Ti | 5.71781 | 2.47241 | 5.54228 |
| Ti | 9.52969 | 2.47241 | 5.54228 |
| Ti | 13.34156 | 2.47241 | 5.54228 |
| Ti | 3.81187 | 7.71594 | 5.54229 |
| Ti | 7.62375 | 7.71594 | 5.54229 |
| Ti | 11.43562 | 7.71594 | 5.54229 |
| Ti | 3.81113 | 9.29409 | 8.35056 |
| Ti | 7.62531 | 9.26745 | 8.30672 |
| Ti | 11.42368 | 9.28712 | 8.34396 |
| Ti | 5.73112 | 4.10054 | 8.27292 |
| Ti | 9.52387 | 4.06077 | 8.32059 |

| | | | |
|---|---|---|---|
| Ti | 13.34154 | 4.02802 | 8.34279 |
| Ti | 5.72448 | 1.19923 | 9.00366 |
| Ti | 9.51886 | 1.20402 | 9.00771 |
| Ti | 13.33515 | 1.18186 | 9.01176 |
| Ti | 3.77817 | 6.43913 | 8.99729 |
| Ti | 7.63679 | 6.43694 | 9.13541 |
| Ti | 11.45134 | 6.43319 | 8.99629 |
| O | 0.00000 | 10.19857 | 0.37332 |
| O | 1.90594 | 4.95504 | 0.37332 |
| O | 1.90594 | 1.98690 | 1.26110 |
| O | 0.00000 | 7.23042 | 1.26110 |
| O | 0.00000 | 3.45367 | 1.83339 |
| O | 1.90594 | 8.69720 | 1.83340 |
| O | 1.90594 | 5.72904 | 2.72118 |
| O | 0.00000 | 0.48552 | 2.72118 |
| O | 0.00000 | 8.81302 | 3.92446 |
| O | 1.90594 | 3.56949 | 3.92446 |
| O | 1.90594 | 0.60134 | 4.81224 |
| O | 0.00000 | 5.84486 | 4.81225 |
| O | 0.00000 | 2.06812 | 5.38454 |
| O | 1.90594 | 7.31164 | 5.38454 |
| O | 1.90594 | 4.34349 | 6.27232 |
| O | 0.00000 | 9.58701 | 6.27232 |
| O | 15.24193 | 7.36565 | 7.45539 |
| O | 1.90752 | 2.12249 | 7.45847 |
| O | 1.90844 | 9.68983 | 8.41243 |
| O | 15.24328 | 4.44212 | 8.39029 |
| O | 15.24417 | 0.63401 | 9.20742 |
| O | 1.89139 | 5.87506 | 9.22036 |
| O | 1.90048 | 2.83762 | 9.83163 |
| O | 15.24295 | 8.08005 | 9.82370 |
| O | 3.81187 | 10.19857 | 0.37332 |
| O | 7.62375 | 10.19857 | 0.37332 |
| O | 11.43562 | 10.19857 | 0.37332 |
| O | 5.71781 | 4.95504 | 0.37332 |
| O | 9.52969 | 4.95504 | 0.37332 |
| O | 13.34156 | 4.95504 | 0.37332 |
| O | 5.71781 | 1.98690 | 1.26110 |
| O | 9.52969 | 1.98690 | 1.26110 |
| O | 13.34156 | 1.98690 | 1.26110 |
| O | 3.81187 | 7.23042 | 1.26110 |
| O | 7.62375 | 7.23042 | 1.26110 |
| O | 11.43562 | 7.23042 | 1.26110 |
| O | 3.81187 | 3.45367 | 1.83339 |
| O | 7.62375 | 3.45367 | 1.83339 |
| O | 11.43562 | 3.45367 | 1.83339 |
| O | 5.71781 | 8.69720 | 1.83340 |
| O | 9.52969 | 8.69720 | 1.83340 |
| O | 13.34156 | 8.69720 | 1.83340 |
| O | 5.71781 | 5.72904 | 2.72118 |
| O | 9.52969 | 5.72904 | 2.72118 |

| | | | |
|---|---|---|---|
| O | 13.34156 | 5.72904 | 2.72118 |
| O | 3.81187 | 0.48552 | 2.72118 |
| O | 7.62375 | 0.48552 | 2.72118 |
| O | 11.43562 | 0.48552 | 2.72118 |
| O | 3.81187 | 8.81302 | 3.92446 |
| O | 7.62375 | 8.81302 | 3.92446 |
| O | 11.43562 | 8.81302 | 3.92446 |
| O | 5.71781 | 3.56949 | 3.92446 |
| O | 9.52969 | 3.56949 | 3.92446 |
| O | 13.34156 | 3.56949 | 3.92446 |
| O | 5.71781 | 0.60134 | 4.81224 |
| O | 9.52969 | 0.60134 | 4.81224 |
| O | 13.34156 | 0.60134 | 4.81224 |
| O | 3.81187 | 5.84486 | 4.81225 |
| O | 7.62375 | 5.84486 | 4.81225 |
| O | 11.43562 | 5.84486 | 4.81225 |
| O | 3.81187 | 2.06812 | 5.38454 |
| O | 7.62375 | 2.06812 | 5.38454 |
| O | 11.43562 | 2.06812 | 5.38454 |
| O | 5.71781 | 7.31164 | 5.38454 |
| O | 9.52969 | 7.31164 | 5.38454 |
| O | 13.34156 | 7.31164 | 5.38454 |
| O | 5.71781 | 4.34349 | 6.27232 |
| O | 9.52969 | 4.34349 | 6.27232 |
| O | 13.34156 | 4.34349 | 6.27232 |
| O | 3.81187 | 9.58701 | 6.27232 |
| O | 7.62375 | 9.58701 | 6.27232 |
| O | 11.43562 | 9.58701 | 6.27232 |
| O | 3.76225 | 7.38559 | 7.45333 |
| O | 7.61545 | 7.37437 | 7.48822 |
| O | 11.47838 | 7.37728 | 7.45002 |
| O | 5.68630 | 2.13271 | 7.45676 |
| O | 9.54788 | 2.12477 | 7.44798 |
| O | 13.33696 | 2.11859 | 7.45653 |
| O | 5.71367 | 9.73134 | 8.39289 |
| O | 9.52358 | 9.69896 | 8.39070 |
| O | 13.33821 | 9.68381 | 8.40050 |
| O | 3.79349 | 4.43748 | 8.39730 |
| O | 7.61841 | 4.46477 | 8.32643 |
| O | 11.44319 | 4.43845 | 8.39265 |
| O | 3.81241 | 0.65077 | 9.22061 |
| O | 7.61992 | 0.66463 | 9.19163 |
| O | 11.42967 | 0.63563 | 9.21112 |
| O | 5.67631 | 5.89960 | 9.10780 |
| O | 9.55187 | 5.90488 | 9.12591 |
| O | 13.34562 | 5.87089 | 9.21589 |
| O | 5.76457 | 2.88410 | 9.83160 |
| O | 9.50475 | 2.86238 | 9.81025 |
| O | 13.34171 | 2.83141 | 9.82741 |
| O | 3.83429 | 8.08664 | 9.82521 |
| O | 7.61642 | 8.14600 | 9.83066 |

| | | | |
|---|---|---|---|
| O | 11.41755 | 8.08240 | 9.82127 |
| O | 7.53735 | 5.59450 | 11.05036 |
| O | 6.00360 | 4.22039 | 11.99759 |
| N | 7.25494 | 7.29653 | 15.75040 |
| C | 6.83197 | 5.23290 | 12.02035 |
| C | 6.93206 | 5.96187 | 13.30882 |
| C | 6.19012 | 5.57823 | 14.43148 |
| C | 7.81521 | 7.04265 | 13.41608 |
| C | 6.40035 | 6.26935 | 15.62474 |
| C | 7.93180 | 7.67548 | 14.65260 |

**Table S4.** XYZ coordinates for the bidentate attachment mode

| ATOM | X | Y | Z |
|---|---|---|---|
| H | 3.61682 | 4.83158 | 13.02992 |
| H | 7.92753 | 4.85972 | 12.99759 |
| H | 3.72973 | 3.91697 | 15.36992 |
| H | 7.86306 | 3.94818 | 15.33782 |
| H | 11.42793 | 8.36903 | 10.80023 |
| Ti | 0.00000 | 1.58260 | 1.10335 |
| Ti | 1.90594 | 6.82612 | 1.10336 |
| Ti | 1.90594 | 3.85797 | 1.99114 |
| Ti | 0.00000 | 9.10149 | 1.99114 |
| Ti | 0.00000 | 0.19704 | 4.65450 |
| Ti | 1.90594 | 5.44057 | 4.65450 |
| Ti | 1.90594 | 2.47241 | 5.54228 |
| Ti | 0.00000 | 7.71594 | 5.54229 |
| Ti | 0.02237 | 9.28529 | 8.34111 |
| Ti | 1.93828 | 4.04224 | 8.34572 |
| Ti | 1.93327 | 1.19082 | 9.00881 |
| Ti | 0.02370 | 6.43366 | 9.00992 |
| Ti | 3.81187 | 1.58260 | 1.10335 |
| Ti | 7.62375 | 1.58260 | 1.10335 |
| Ti | 11.43562 | 1.58260 | 1.10335 |
| Ti | 5.71781 | 6.82612 | 1.10336 |
| Ti | 9.52969 | 6.82612 | 1.10336 |
| Ti | 13.34156 | 6.82612 | 1.10336 |
| Ti | 5.71781 | 3.85797 | 1.99114 |
| Ti | 9.52969 | 3.85797 | 1.99114 |
| Ti | 13.34156 | 3.85797 | 1.99114 |
| Ti | 3.81187 | 9.10149 | 1.99114 |
| Ti | 7.62375 | 9.10149 | 1.99114 |
| Ti | 11.43562 | 9.10149 | 1.99114 |
| Ti | 3.81187 | 0.19704 | 4.65450 |
| Ti | 7.62375 | 0.19704 | 4.65450 |
| Ti | 11.43562 | 0.19704 | 4.65450 |
| Ti | 5.71781 | 5.44057 | 4.65450 |
| Ti | 9.52969 | 5.44057 | 4.65450 |
| Ti | 13.34156 | 5.44057 | 4.65450 |
| Ti | 5.71781 | 2.47241 | 5.54228 |
| Ti | 9.52969 | 2.47241 | 5.54228 |

| | | | |
|---|---|---|---|
| Ti | 13.34156 | 2.47241 | 5.54228 |
| Ti | 3.81187 | 7.71594 | 5.54229 |
| Ti | 7.62375 | 7.71594 | 5.54229 |
| Ti | 11.43562 | 7.71594 | 5.54229 |
| Ti | 3.82268 | 9.25054 | 8.30043 |
| Ti | 7.59781 | 9.25406 | 8.29808 |
| Ti | 11.42609 | 9.38471 | 8.23403 |
| Ti | 5.69928 | 4.06566 | 8.23657 |
| Ti | 9.47024 | 4.03395 | 8.33921 |
| Ti | 13.39406 | 4.03048 | 8.34146 |
| Ti | 5.70929 | 1.21991 | 9.01630 |
| Ti | 9.48628 | 1.19225 | 9.01272 |
| Ti | 13.36809 | 1.18552 | 9.01216 |
| Ti | 3.86375 | 6.43231 | 9.13226 |
| Ti | 7.57327 | 6.42649 | 9.11876 |
| Ti | 11.43171 | 6.30161 | 8.93489 |
| O | 0.00000 | 10.19857 | 0.37332 |
| O | 1.90594 | 4.95504 | 0.37332 |
| O | 1.90594 | 1.98690 | 1.26110 |
| O | 0.00000 | 7.23042 | 1.26110 |
| O | 0.00000 | 3.45367 | 1.83339 |
| O | 1.90594 | 8.69720 | 1.83340 |
| O | 1.90594 | 5.72904 | 2.72118 |
| O | 0.00000 | 0.48552 | 2.72118 |
| O | 0.00000 | 8.81302 | 3.92446 |
| O | 1.90594 | 3.56949 | 3.92446 |
| O | 1.90594 | 0.60134 | 4.81224 |
| O | 0.00000 | 5.84486 | 4.81225 |
| O | 0.00000 | 2.06812 | 5.38454 |
| O | 1.90594 | 7.31164 | 5.38454 |
| O | 1.90594 | 4.34349 | 6.27232 |
| O | 0.00000 | 9.58701 | 6.27232 |
| O | 15.24498 | 7.36923 | 7.45595 |
| O | 1.90942 | 2.12436 | 7.45284 |
| O | 1.89186 | 9.69972 | 8.39560 |
| O | 15.24174 | 4.44669 | 8.38538 |
| O | 15.24149 | 0.63411 | 9.21401 |
| O | 1.90176 | 5.88329 | 9.18592 |
| O | 1.89216 | 2.84055 | 9.82631 |
| O | 15.23963 | 8.08439 | 9.82689 |
| O | 3.81187 | 10.19857 | 0.37332 |
| O | 7.62375 | 10.19857 | 0.37332 |
| O | 11.43562 | 10.19857 | 0.37332 |
| O | 5.71781 | 4.95504 | 0.37332 |
| O | 9.52969 | 4.95504 | 0.37332 |
| O | 13.34156 | 4.95504 | 0.37332 |
| O | 5.71781 | 1.98690 | 1.26110 |
| O | 9.52969 | 1.98690 | 1.26110 |
| O | 13.34156 | 1.98690 | 1.26110 |
| O | 3.81187 | 7.23042 | 1.26110 |
| O | 7.62375 | 7.23042 | 1.26110 |

| | | | |
|---|---|---|---|
| O | 11.43562 | 7.23042 | 1.26110 |
| O | 3.81187 | 3.45367 | 1.83339 |
| O | 7.62375 | 3.45367 | 1.83339 |
| O | 11.43562 | 3.45367 | 1.83339 |
| O | 5.71781 | 8.69720 | 1.83340 |
| O | 9.52969 | 8.69720 | 1.83340 |
| O | 13.34156 | 8.69720 | 1.83340 |
| O | 5.71781 | 5.72904 | 2.72118 |
| O | 9.52969 | 5.72904 | 2.72118 |
| O | 13.34156 | 5.72904 | 2.72118 |
| O | 3.81187 | 0.48552 | 2.72118 |
| O | 7.62375 | 0.48552 | 2.72118 |
| O | 11.43562 | 0.48552 | 2.72118 |
| O | 3.81187 | 8.81302 | 3.92446 |
| O | 7.62375 | 8.81302 | 3.92446 |
| O | 11.43562 | 8.81302 | 3.92446 |
| O | 5.71781 | 3.56949 | 3.92446 |
| O | 9.52969 | 3.56949 | 3.92446 |
| O | 13.34156 | 3.56949 | 3.92446 |
| O | 5.71781 | 0.60134 | 4.81224 |
| O | 9.52969 | 0.60134 | 4.81224 |
| O | 13.34156 | 0.60134 | 4.81224 |
| O | 3.81187 | 5.84486 | 4.81225 |
| O | 7.62375 | 5.84486 | 4.81225 |
| O | 11.43562 | 5.84486 | 4.81225 |
| O | 3.81187 | 2.06812 | 5.38454 |
| O | 7.62375 | 2.06812 | 5.38454 |
| O | 11.43562 | 2.06812 | 5.38454 |
| O | 5.71781 | 7.31164 | 5.38454 |
| O | 9.52969 | 7.31164 | 5.38454 |
| O | 13.34156 | 7.31164 | 5.38454 |
| O | 5.71781 | 4.34349 | 6.27232 |
| O | 9.52969 | 4.34349 | 6.27232 |
| O | 13.34156 | 4.34349 | 6.27232 |
| O | 3.81187 | 9.58701 | 6.27232 |
| O | 7.62375 | 9.58701 | 6.27232 |
| O | 11.43562 | 9.58701 | 6.27232 |
| O | 3.74459 | 7.40033 | 7.47311 |
| O | 7.69831 | 7.40163 | 7.46546 |
| O | 11.44016 | 7.40442 | 7.49458 |
| O | 5.71345 | 2.11073 | 7.42993 |
| O | 9.52234 | 2.12215 | 7.45360 |
| O | 13.35257 | 2.12271 | 7.45672 |
| O | 5.72001 | 9.68308 | 8.38897 |
| O | 9.55275 | 9.70906 | 8.38366 |
| O | 13.33143 | 9.69929 | 8.38174 |
| O | 3.79949 | 4.40252 | 8.40996 |
| O | 7.63857 | 4.40033 | 8.40033 |
| O | 11.45053 | 4.48318 | 8.33774 |
| O | 3.81278 | 0.66010 | 9.18850 |
| O | 7.62408 | 0.65852 | 9.19490 |

| | | | |
|---|---|---|---|
| O | 11.44133 | 0.61933 | 9.21766 |
| O | 5.72302 | 5.98643 | 8.61406 |
| O | 9.54821 | 5.86853 | 9.19724 |
| O | 13.34019 | 5.86775 | 9.22658 |
| O | 5.71833 | 2.87128 | 9.78435 |
| O | 9.54943 | 2.84180 | 9.82760 |
| O | 13.34077 | 2.84036 | 9.82691 |
| O | 3.81114 | 8.13720 | 9.82112 |
| O | 7.64695 | 8.13616 | 9.81170 |
| O | 11.44184 | 8.06608 | 9.87828 |
| O | 6.88313 | 5.77344 | 10.93841 |
| O | 4.60363 | 5.76646 | 10.95584 |
| C | 5.74677 | 5.52751 | 11.47675 |
| C | 5.76805 | 4.92873 | 12.84625 |
| C | 4.57343 | 4.64719 | 13.51709 |
| C | 6.97918 | 4.66502 | 13.49719 |
| C | 4.64461 | 4.13582 | 14.81325 |
| C | 6.93620 | 4.15335 | 14.79493 |
| N | 5.79751 | 3.89385 | 15.45708 |