

## Supplementary Data

This supplementary data is a part of a paper entitled “Computational Study of Photosynthetic Pigments: Toward Synthetic Photosynthesis Engineering”.

**Table S1.** Time-dependent DFT results (no solvent) and converted FMO energy gap of the 1<sup>st</sup> excitation state

| Pigment | Excited state | Energy (eV) | Wavelength (nm) | Oscillator strength (f) | Transition details                                                                                 |
|---------|---------------|-------------|-----------------|-------------------------|----------------------------------------------------------------------------------------------------|
| Chl a   | 1             | 2.1816      | 568.32          | 0.2913                  | H-1→L: -0.21241; H-1→L+1: -0.17841; H→L: 0.62942; H→L+1: -0.13813                                  |
|         | 2             | 2.4526      | 505.52          | 0.0906                  | H-1→L: 0.58240; H→L: 0.24861; H→L+1: 0.28224                                                       |
|         | 3             | 3.3222      | 373.20          | 0.0610                  | H-2→L: 0.63939; H-2→L+1: -0.16662; H-1→L: 0.11946; H→L+1: -0.12092                                 |
| Chl b   | 1             | 2.1376      | 580.03          | 0.2403                  | H-1→L: -0.19705; H-1→L+1: -0.19668; H→L: 0.62091; H→L+1: -0.15330                                  |
|         | 2             | 2.4438      | 507.35          | 0.0595                  | H-1→L: 0.55330; H→L: 0.24779; H→L+1: 0.32612; H→L+2: 0.11411                                       |
|         | 3             | 3.1836      | 389.45          | 0.7274                  | H-4→L: 0.16392; H-2→L: -0.13671; H-1→L: -0.34680; H→L+1: 0.56180                                   |
| Chl c   | 1             | 2.3979      | 517.06          | 0.0240                  | H-1→L+1: 0.37652; H→L: 0.56172                                                                     |
|         | 2             | 2.5487      | 486.46          | 0.0343                  | H-1→L: 0.54320; H→L: -0.10095; H→L+1: -0.41548                                                     |
|         | 3             | 2.8032      | 442.29          | 0.0231                  | H-1→L: 0.16155; H→L+1: 0.13442; H→L+2: 0.66266                                                     |
| Chl d   | 1             | 2.2946      | 540.33          | 0.1687                  | H-1→L: 0.43567; H-1→L+1: 0.12106; H-1→L+2: 0.11678; H→L: 0.46317; H→L+1: -0.11385; H→L+2: -0.20847 |
|         | 2             | 2.4336      | 509.47          | 0.1420                  | H-1→L: -0.42911; H-1→L+1: 0.10500; H→L: 0.46354; H→L+1: 0.22675; H→L+2: 0.11402                    |
|         | 3             | 2.5115      | 493.67          | 0.0245                  | H-1→L: 0.20496; H→L+1: 0.65357; H→L+2: -0.12751                                                    |
| Chl f   | 1             | 0.3367      | 3682.40         | 0.0016                  | H→L: 0.69994                                                                                       |
|         | 2             | 1.8093      | 685.27          | 0.1252                  | H-1→L: -0.11693; H→L+1: 0.68223                                                                    |
|         | 3             | 2.0234      | 612.76          | 0.1700                  | H-1→L: 0.67954; H→L+1: 0.12039                                                                     |
| BChl a  | 1             | 1.5665      | 791.49          | 0.3580                  | H-1→L+1: 0.14020; H→L: 0.69417                                                                     |
|         | 2             | 2.3218      | 534.00          | 0.0834                  | H-1→L: 0.62560; H→L+1: -0.31240                                                                    |
|         | 3             | 3.3278      | 372.57          | 0.0015                  | H-2→H: 0.68326                                                                                     |
| BChl b  | 1             | 1.5373      | 806.51          | 0.3543                  | H-1→L+1: 0.13622; H→L: 0.69532                                                                     |
|         | 2             | 2.3163      | 535.28          | 0.0933                  | H-1→L: 0.63118; H→L+1: -0.30299                                                                    |
|         | 3             | 3.2653      | 379.71          | 0.0051                  | H-2→L: 0.68232                                                                                     |
| BChl c  | 1             | 1.7982      | 689.50          | 0.0509                  | H-4→L: -0.15726; H-2→L: -0.11822; H-2→L+1: 0.10326; H-1→L: 0.56745; H→L: 0.31741                   |
|         | 2             | 2.1952      | 564.79          | 0.0104                  | H-2→L: 0.51439; H-1→L+1: -0.38057; H→L+1: -0.21485                                                 |
|         | 3             | 2.8766      | 431.00          | 0.0233                  | H-4→L: 0.51933; H-2→L+1: 0.41471                                                                   |
| BChl d  | 1             | 0.2245      | 5521.90         | 0.0070                  | H→L: 0.79786; H→L+1: 0.13742; H→L: -0.40771                                                        |
|         | 2             | 0.9363      | 1324.16         | 0.0065                  | H→L: -0.12792; H→L+1: 0.68394                                                                      |
|         | 3             | 1.5094      | 821.43          | 0.2236                  | H-1→L: 0.67855; H-1→L+1: 0.14717; H→L: -0.10867                                                    |
| BChl e  | 1             | 0.4743      | 2613.92         | 0.0089                  | H-1→L: 0.15265; H→L: 0.68271; H→L+1: -0.12565; H→L: -0.11924                                       |
|         | 2             | 1.4476      | 856.47          | 0.0451                  | H-2→L: 0.11462; H-1→L: 0.61398; H-1→L+1: -0.11087; H→L: -0.18506; H→L+1: -0.20955                  |
|         | 3             | 2.0197      | 613.87          | 0.0003                  | H-2→L: 0.58254; H→L+1: 0.34002                                                                     |
| BChl g  | 1             | 2.2129      | 560.27          | 0.2862                  | H-1→L+1: 0.10779; H→L: 0.69559                                                                     |
|         | 2             | 2.6153      | 474.07          | 0.1210                  | H-5→L: -0.13148; H-1→L: 0.62470; H→L+1: -0.28412                                                   |
|         | 3             | 3.4308      | 361.39          | 0.0081                  | H-5→L: 0.62955; H-4→L: 0.16766; H→L+1: -0.20939                                                    |

**Table S2.** Time-dependent DFT results (SMD, H<sub>2</sub>O) and converted FMO energy gap of the 1st excitation state

| Pigment | Excited state | Energy (eV) | Wavelength (nm) | Oscillator strength (f) | Transition Details                                                                  |
|---------|---------------|-------------|-----------------|-------------------------|-------------------------------------------------------------------------------------|
| Chl a   | 1             | 2.1450      | 578.02          | 0.3811                  | H-1→L: -0.28269; H-1→L+1: -0.14934; H→L: 0.60580; H→L+1: -0.15156                   |
|         | 2             | 2.3918      | 518.38          | 0.2024                  | H-1→L: 0.59145; H→L: 0.31195; H→L+1: 0.18389                                        |
|         | 3             | 3.3328      | 372.01          | 0.6463                  | H-5→L: 0.19370; H-1→L: -0.21141; H-1→L+2: 0.12944; H→L+1: 0.61619                   |
| Chl b   | 1             | 2.0797      | 596.15          | 0.3325                  | H-1→L: -0.23388; H-1→L+1: -0.17330; H→L: 0.61667; H→L+1: -0.14936                   |
|         | 2             | 2.3868      | 519.45          | 0.1684                  | H-1→L: 0.59488; H→L: 0.27442; H→L+1: 0.21925; H→L+2: 0.10927                        |
|         | 3             | 3.0763      | 403.03          | 0.7435                  | H-4→L: 0.14145; H-1→L: -0.24448; H-1→L+1: -0.15098; H→L+1: 0.62151                  |
| Chl c   | 1             | 2.3568      | 526.07          | 0.0960                  | H-1→L: 0.13051; H-1→L+1: 0.29058; H→L: 0.59720; H→L+1: -0.13455                     |
|         | 2             | 2.5829      | 480.02          | 0.0632                  | H-1→L: 0.55207; H→L: -0.16450; H→L+1: -0.37814                                      |
|         | 3             | 3.1715      | 390.93          | 0.8896                  | H-2→L: -0.18368; H-1→L: 0.38600; H→L+1: 0.53074                                     |
| Chl d   | 1             | 2.2272      | 556.67          | 0.2321                  | H-1→L: 0.63528; H→L: -0.17898; H→L+1: 0.22003                                       |
|         | 2             | 2.3762      | 521.77          | 0.3181                  | H-1→L: 0.19682; H-1→L+1: -0.11712; H→L: 0.65734                                     |
|         | 3             | 3.3354      | 371.73          | 0.4111                  | H-5→L: 0.19895; H-1→L: -0.15257; H-1→L+1: -0.31144; H→L+1: 0.55281                  |
| Chl f   | 1             | 1.1472      | 1080.71         | 0.0104                  | H→L: 0.69395                                                                        |
|         | 2             | 2.1774      | 569.43          | 0.1804                  | H-1→L: 0.68320; H-1→L+1: 0.10674                                                    |
|         | 3             | 2.4425      | 507.61          | 0.3569                  | H→L+1: 0.67802; H→L+2: -0.13334                                                     |
| BChl a  | 1             | 1.4175      | 874.65          | 0.4872                  | H-1→L+1: 0.10517; H→L: 0.69795                                                      |
|         | 2             | 2.2295      | 556.10          | 0.1572                  | H-1→L: 0.65254; H→L+1: -0.24349                                                     |
|         | 3             | 3.2679      | 379.40          | 0.6510                  | H-1→L: 0.23672; H→L+1: 0.65811                                                      |
| BChl b  | 1             | 1.4042      | 882.98          | 0.4793                  | H-1→L+1: 0.10936; H→L: 0.69812                                                      |
|         | 2             | 2.2274      | 556.63          | 0.1683                  | H-1→L: 0.65645; H→L+1: -0.24156                                                     |
|         | 3             | 3.2868      | 377.22          | 0.0483                  | H-5→L: -0.24681; H-2→L: 0.62240; H→L+1: -0.14213                                    |
| BChl c  | 1             | 1.7975      | 689.75          | 0.0855                  | H-4→L: -0.14203; H-2→L: -0.12806; H-2→L+1: 0.10062; H-1→L: 0.65164                  |
|         | 2             | 2.2061      | 562.01          | 0.0248                  | H-2→L: 0.53702; H-1→L+1: -0.40377                                                   |
|         | 3             | 2.8485      | 435.26          | 0.7914                  | H-4→L: 0.16212; H→L: 0.55448; H→L+1: 0.22724; H→L+2: -0.27731                       |
| BChl d  | 1             | 0.6548      | 1893.48         | 0.0269                  | H→L: 0.70256                                                                        |
|         | 2             | 1.7875      | 693.61          | 0.3791                  | H-1→L: 0.69573                                                                      |
|         | 3             | 2.0344      | 609.44          | 0.0368                  | H-1→L+1: 0.22817; H→L+1: 0.64908                                                    |
| BChl e  | 1             | 0.6471      | 1915.89         | 0.0134                  | H-1→L: 0.19230; H→L: 0.66571; H→L+1: 0.10449                                        |
|         | 2             | 1.4530      | 853.31          | 0.0957                  | H-1→L: 0.62702; H→L: -0.21381; H→L+1: 0.18201                                       |
|         | 3             | 2.2552      | 549.77          | 0.0003                  | H-6→L: -0.15344; H-4→L: -0.14002; H-3→L: 0.56094; H-1→L+1: 0.12487; H→L+1: -0.29423 |
| BChl g  | 1             | 2.4484      | 506.39          | 0.3766                  | H→L: 0.69651                                                                        |
|         | 2             | 2.5934      | 478.07          | 0.2365                  | H-3→L: -0.15073; H-1→L: 0.64877; H→L+1: -0.21186                                    |
|         | 3             | 3.3494      | 370.17          | 0.0424                  | H-3→L: 0.66470; H-1→L: 0.11216; H→L+1: -0.14687                                     |