**Supplementary Table 6**. TD-DFT/MM emissions corresponding to the electronic transition between S1 and S0 for GBAv-open and GBAv-closed. The TD-DFT/MM calculations were performed with the 6-311G(2d,p) basis set and the B3LYP functional on a structure optimized at the same level of theory.

|  |  |  |
| --- | --- | --- |
| Model (numbering of the snapshot)*a* | TD-DFT/MM emission transition in eV*b* | Experimental value for GBAv in eV*b* |
| GBAv-open (1) | 2.24 (552) | 2.3 (538) |
| GBAv-open (2) | 2.25 (551) |
| GBAv-open (3) | 2.24 (553) |
| GBAv-open (4) | 2.29 (541) |
| GBAv-closed (1) | 2.32 (535) |
| GBAv-closed (2) | 2.33 (532) |
| GBAv-closed (3) | 2.36 (525) |
| GBAv-closed (4) | 2.35 (527) |

*a*The values in parentheses represent the number of the snapshot extracted from the corresponding MD simulation.

*b*The associated wavelengths in nm are given in parentheses.