Supporting Information

Mechanism of High Photoluminescence Quantum Yield of Melem

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XRD analysis was conducted using a diffractometer (Ultima IV, Rigaku) with a Cu Kα radiation source (λ = 0.15496 nm).

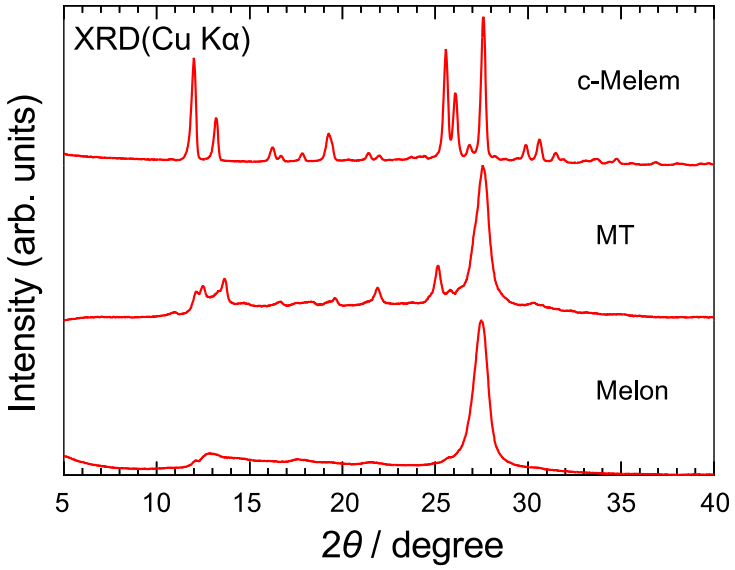


Fig. S1. XRD profiles of c-melem, MT, and melon. The melon and MT samples are the same samples as in the previous study.[1]

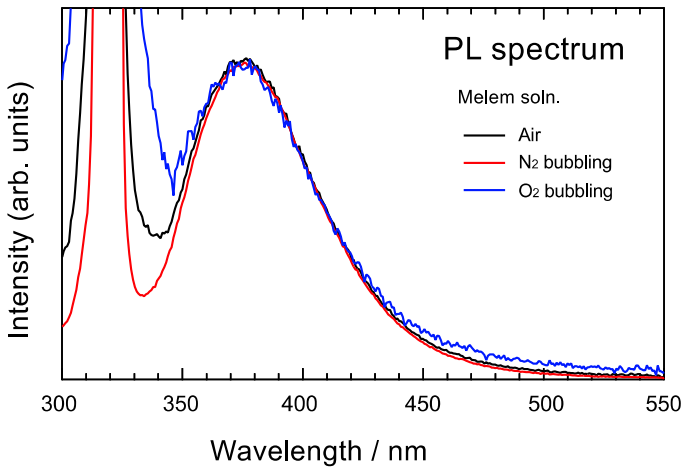
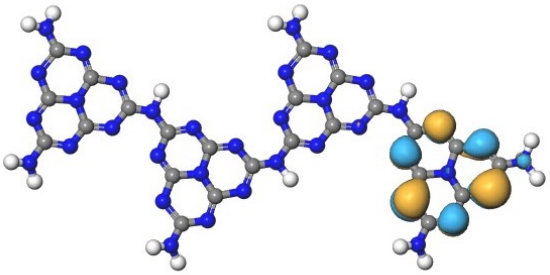
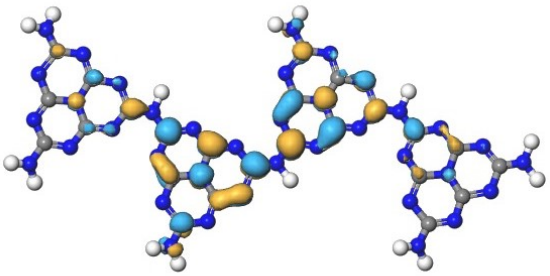


Fig. S2. PL spectra of air, N_2 bubbling, and O_2 bubbling melem solution samples. The vertical axis represents the PL emission intensity, with the peak at 320 nm because of photoexcitation. The data are the same as in Figure 3(b), but normalized by the intensity of the 376 nm peak.



HOMO − 4



LUMO

Fig. S3. Wave functions of the HOMO-4 and LUMO of MT simulated by DFT calculation. The blue and yellow parts represent different wavefunction signs. The lowest-energy emission from MT is caused by transitions between these two orbitals.

1 Y. Miyake, G. Seo, K. Matsuhashi, N. Takada and K. Kanai, *Materials Advances*, 2021, **2**, 6083–6093.