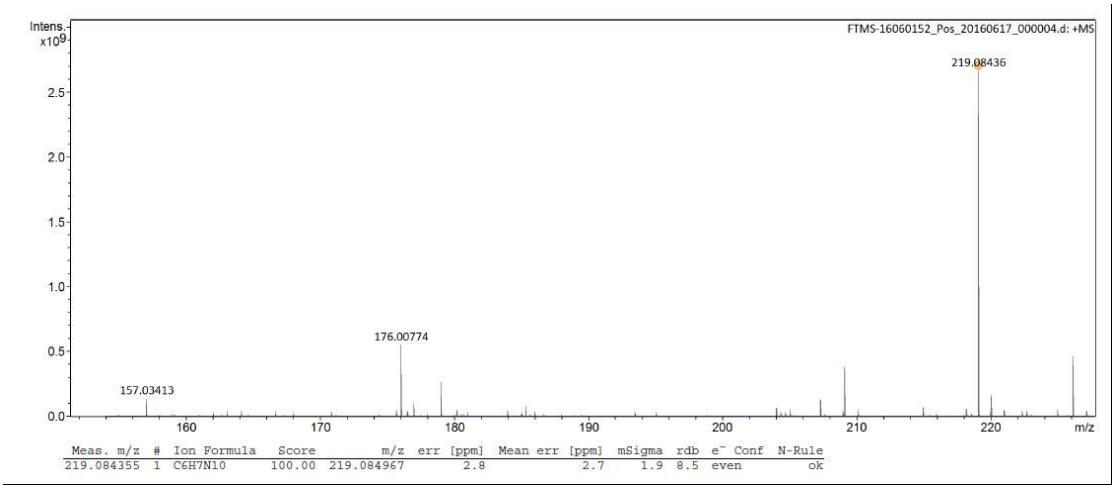


Fig. S1 Mass spectrometry of Melem.

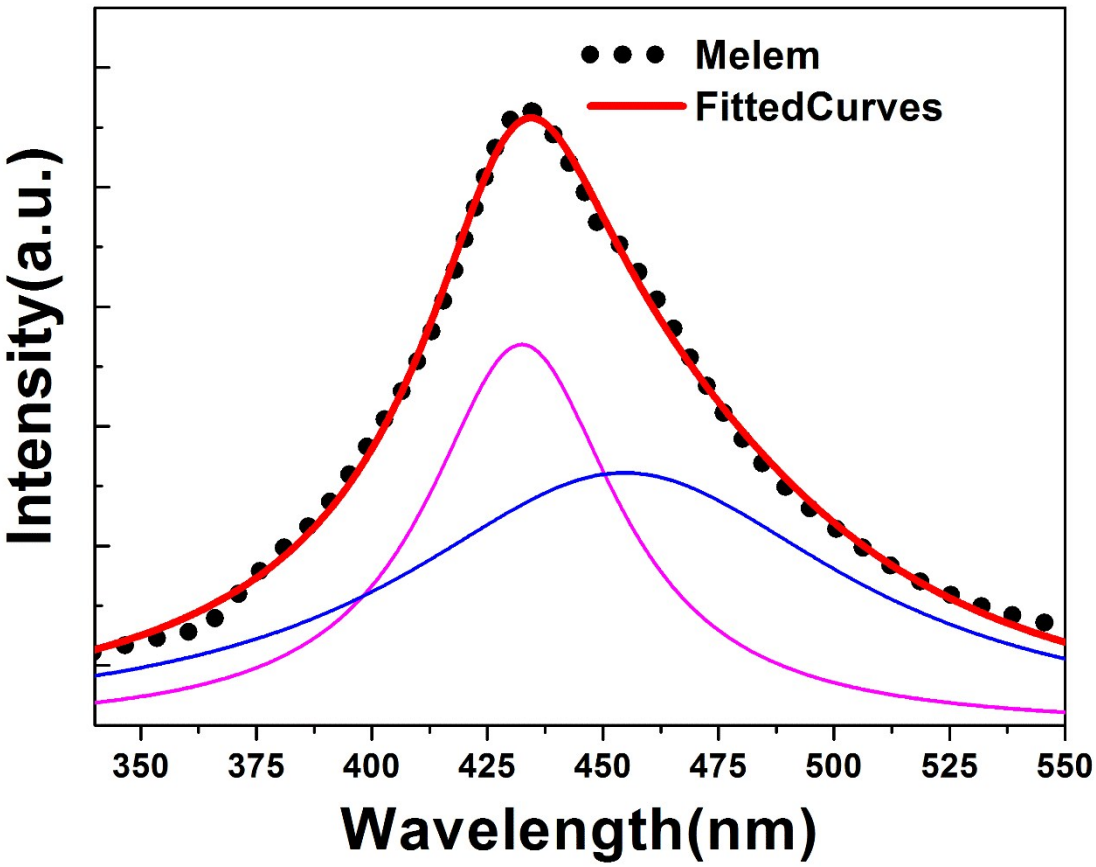
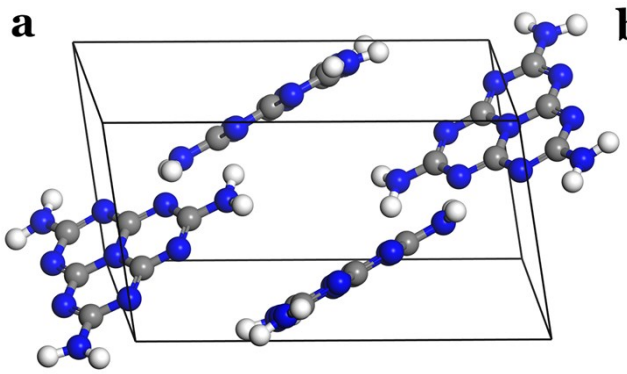


Fig. S2 Lorenz fitting of the emission spectra of melem under the excitation of 320nm



Formula	$C_6N_7(NH_2)_3$
Crystal system	Monoclinic
Space group	P21/c
γ/deg	90.0000
a/Å	7.3992
b/Å	8.6528
c/Å	13.3816

Fig. S3 (a) Crystal structure of melem and (b) lattice constants of melem.

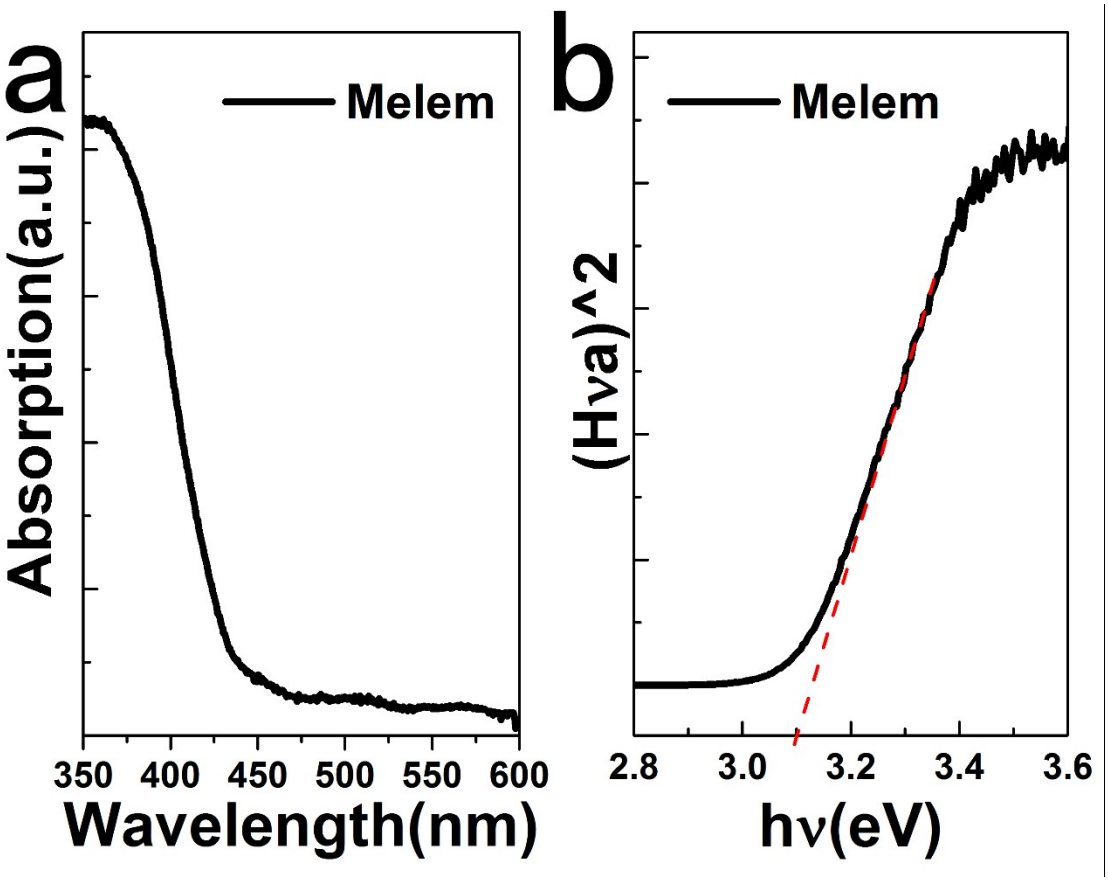


Fig. S4 (a) the optical absorption spectrum of melem and (b) the calculated band gap of melem

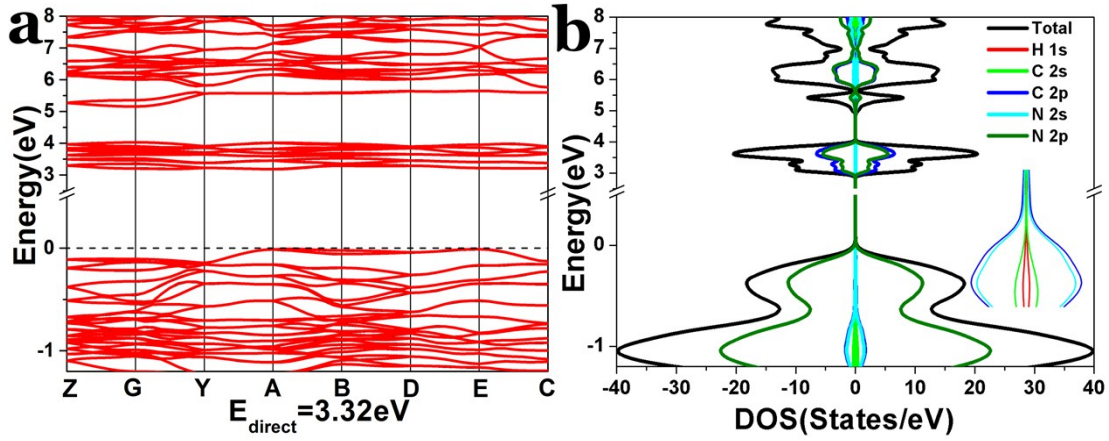


Fig. S5 (a) band structure and (b) DOS of melem calculated by using HSE when AEXX =0.01.

The band structure and DOS were calculated by using the spin Heyd-Scuseria-Ernzerhof (HSE) functional to represent the electronic exchange-correlation energy. For melem unit cell, cut-off energy and Monkhorst-Pack k-point mesh were 500 eV and 3×3×2, respectively. The structural relaxations were performed until the self-consistent total energy difference reached 10^{-4} eV and the residual forces on atoms fell below 0.01 eV·Å^{-1}. The effects of spin polarization were considered in energy calculations.