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Tuning the band structures of self-activated luminescence materials for white- emission and biological application. JUNYING ZHANG, BeiHang University — The properties of the self-activated luminescence materials depend closely on the point defects, crystal size and even shape. Using first-principles calculation, we exploit the influence of oxygen vacancy on the band structure of monoclinic Y_2WO_6 . Then by controlling the calcining process and doping with some rare earth elements, strong green emission and also white-emission could be achieved under long-wavelength violet light irradiation. For graphitic- phase C_3N_4 (g-C_3N_4), bright blue emission was obtained by delamination of the bulk materials and reducing the crystal size. By further reducing the particle to about 5nm, water-dispersible g-C_3N_4 quantum dots were produced which show potential application as photodynamic therapy agent. The pH-sensitive emission of g-C_3N_4 deduces the high cytotoxicity to cancer cell and low cytotoxicity to the normal cell of g-C_3N_4-porphyrin.

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