Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information

Extraction of surface trap level from photoluminescence: A case study of ZnO nanostructures

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1. Characterization of the pleated ZnO nanosheets.

The Mg content in the nanosheets is below the detection limit of EDS (Energy dispersive spectroscopy).

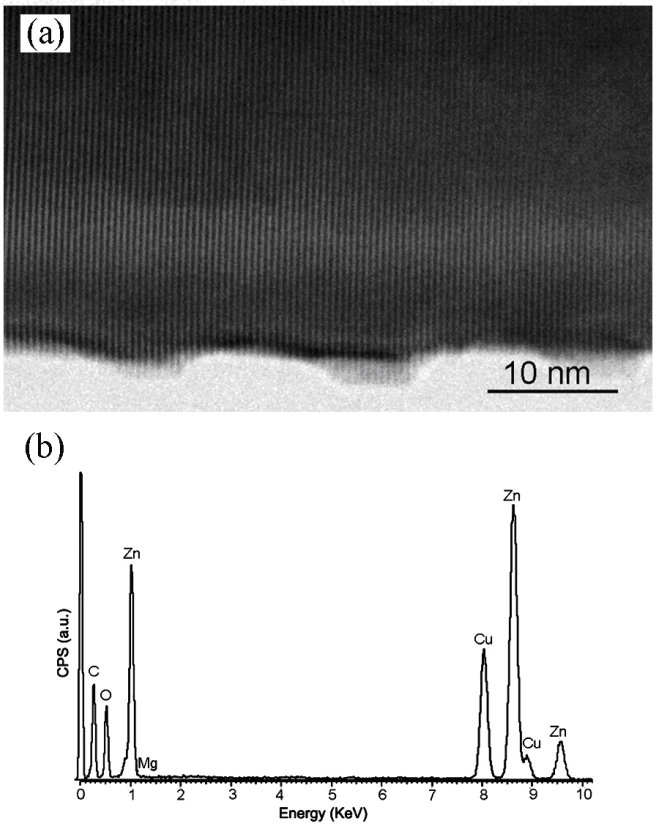

Figure S1. (a) High resolution TEM image of the pleated ZnO nanosheets. (b) EDS of the pleated ZnO nanosheets. The position of Mg (1.2 KeV) is indicated in the spectrum. The Mg content is below the detection limit. Note the EDS is attached to TEM and Cu and C is from the Cu grid with carbon film.

2. Temperature-dependent photoluminescence of ZnO nanorods for comparison.

To confirm the role of surface states in the negative thermal quenching (NTQ), PL properties of ZnO nanorods with relatively large diameter were studied. Figure S2(a) shows the morphology of a typical nanorods sample with diameter varying between 300 and 400 nm. Its low temperature PL (Figure S2(b)) shows well resolved free exciton (FX) emission at 3.377 eV and donor bound exciton (D^0X) emission at 3.362 eV. The linewidth is ~10 meV, much smaller than that of surface exciton in pleated nanosheets. The absence of surface exciton emission and the small linewidth of the excitonic emissions are indicative of much lower density of surface states in the nanorods.

The emission near 3.31 eV is known as the *A* line, which is usually attributed to transition involving stacking faults[1] in the basal plane or the longitudinal optical (LO) phonon replica of the free exciton.[2]

The thermal quenching of PL in ZnO nanorods is plotted in Figure S3. It is clear that both the excitonic and green emissions show normal thermal quenching feature, which can be described in terms of thermal activation of nonradiative recombination rates.[3]

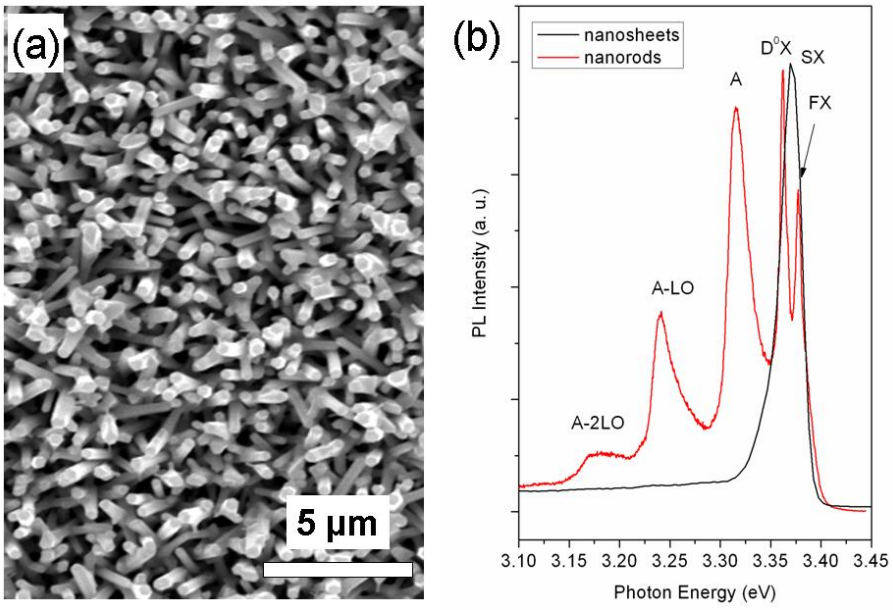

Figure S2. (a) SEM image of ZnO nanords; (b) low temperature PL spectra of pleated ZnO nanosheets and ZnO nanorods. The intensities are normalized to the SX and D^0X.

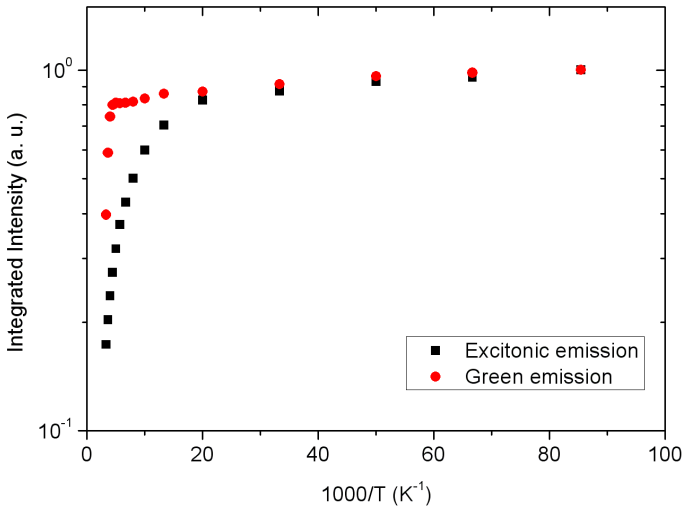

Figure S3. Normal thermal quenching of the excitonic and green emissions in ZnO nanorods.

References

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3. J. Krustok, H. Collan, and K. Hjelt, *J. Appl. Phys.*, 1997, **81**, 1442.