Role of Defects in Optical Properties of 2D h-BN

Junkai Ren
Luigi Stagi, Luca Malfatti, and Plinio Innocenzi

Laboratory of Materials Science and Nanotechnology, Department of Chemistry and Pharmacy, CR-INSTM, University of Sassari, Via Vienna 2, 07100, Sassari, Italy

E-mail: j.ren@studenti.uniss.it

Abstract

Two-dimensional hexagonal boron nitride (2D h-BN) is representing one of the most popular layered materials whose excellent properties are expected to have great potentials in optics and electronics.[1-2] The introduction of tailored defects can endow 2D h-BN with many new properties, such as fluorescence and photocatalytic activity.[3-4] Therefore, managing defects in h-BN is a key process to exploit its advanced functions. However, a clear correspondence between defects and properties still has not been well established in terms of h-BN basic research.

In this report, h-BN nanosheets (h-BNNSs) have been prepared by sonication-assisted liquid-phase exfoliation of the bulk powders. In one hand, the exfoliation in water can make cavitation and allow producing hydroxyl-defective h-BNNSs which show a visible photoluminescence (**Figure 1a**).[5] In another hand, the exfoliation in N-methyl-2-pyrrolidone (NMP) only produces relatively defect-free h-BNNSs, consequently, without that visible fluorescence. It highlights the critical role of hydroxylation and oxidation in the fluorescent emission as well as the rising optical absorbance of the 2D h-BN structure. Subsequently, the nanosheets have been successfully incorporated into titania (TiO_2) mesoporous films to form heterostructures via a template-assisted self-assembly (**Figure 1b**).[6] Both bare and defective BN sheets do not show photocatalytic properties but can contribute to the anatase TiO_2 crystallization by heterogeneous nucleation. Importantly, the defects of h-BNNSs can further increase the UVA absorbance and thereby enhance the photocatalytic response of the film.

In a summary, defective h-BNNSs can be prepared via sonication-assisted exfoliation of their bulk counterpart in water-phase. The tailored defects not only can induce visible emission from h-BN layer but also enhance the photocatalytic property of BN-TiO_2 heterojunction. Prospectively, only through a better understanding of multiple defects, it is possible to create new properties of h-BN materials and develop their advanced functions.

References

[1] **J. Ren**, L. Stagi, P. Innocenzi *J. Mater. Sci.*, 56 (2021) 4053.
[2] L. Stagi, **J. Ren**, P. Innocenzi. *Materials*, 12 (2019) 3905.
[3] **J. Ren**, P. Innocenzi. *Small Struct.*, 2 (2021) 2100068.
[4] **J. Ren**, L. Stagi, L. Malfatti, C. M. Carbonaro, G. Granozzi, L. Calvillo, S. Garroni, S. Enzo, P. Innocenzi. *Appl. Surf. Sci.*, 567 (2021) 150727.
[5] **J. Ren**, Luigi Stagi, C. M. Carbonaro, L. Malfatti, M. F. Casula, P. C. Ricci, A. D. Rio, F. Bonaccorso, L. Calvillo, G. Granozzi, P. Innocenzi. *2D Mater.*, 7 (2020) 045023.
[6] **J. Ren**, L. Stagi, L. Malfatti, S. Garroni, S. Enzo, P. Innocenzi. *Langmuir*, 37 (2021) 5348.

Figures

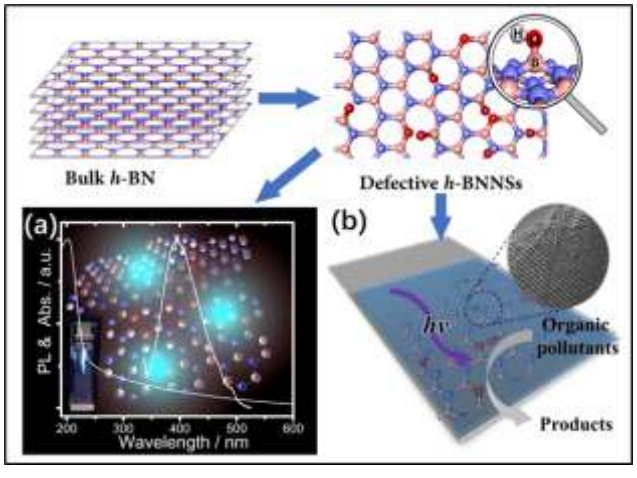

Figure 1: Defect-assisted (a) luminescence from h-BNNSs and (b) enhanced photocatalysis in BN-TiO_2 film heterostructure.