Single-photon emission from defects in hexagonal boron nitride: A computational study

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Point defects in sheets of hexagonal boron nitride have recently been studied as potential single-photon emitters: Experimental studies have shown that the emission from point defect color centers has extremely narrow bandwidth and mainly takes place in the zero phonon line[1][2].
From an engineering perspective, a high-quality source of single photons would be extremely useful for many applications including quantum computing and quantum communications.
Currently, it is not clear which defect systems in boron nitride have the right properties for use as single-photon emitters. Different experimental studies have observed significantly different emission energies, indicating that multiple different defect states can produce single photons.
More investigations are thus needed to understand which properties of defects are important for single-photon emission, and which properties of boron nitride make it suitable as host. We have used density functional theory to explore the potential energy surfaces of the ground- and lowest excited states around different point defects in hBN. Our calculations shed light on the observed narrow band nature of the emission lines and indicate potential routes for tuning emission energy, line width and lifetime.

References

[1] Tran, Bray, Ford, Toth, Aharonovich, Nat. Nano., 11 (2016) 37-41
[2] Vuong, Cassabois, Valvin, Ouerghi, Chassagneux, Voisin, Gil, PRL 117 (2016) 097402

Figures

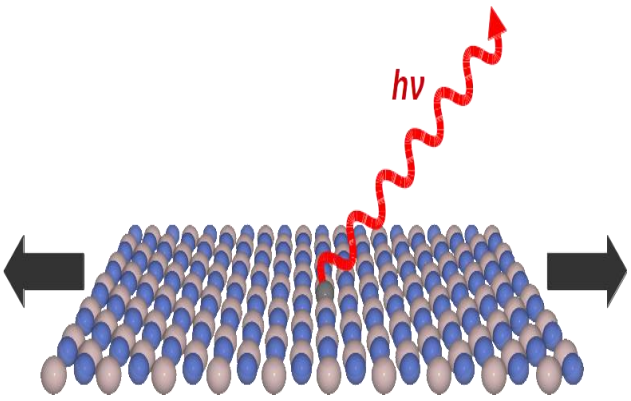

Figure 1: Light emission from a color center in boron nitride.