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Defects in Two Dimensional Crystals: An Ultra-high Resolution Aberration-corrected Electron Microscopy Study

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Graphene and hexagonal boron nitride (h-BN) are considered new emerging materials with potential applications in sensing [1], hydrogen storage [2], and electronics [3]. The configuration of defects and edges in these crystals can have a significant impact on their resulting physical, chemical and electronic properties. In addition, small distortions in the atomic structure of such crystal membranes can lead to peculiar physical, chemical and electronic properties at the bulk. As a result, nanoscale engineering of such crystals is very crucial to tailor their large scale properties. During the past decade, aberration-corrected ultra-high resolution electron microscopy has revolutionized our understanding of the nanoscale phenomena by opening up the possibility of imaging every single atom or atomic column within a crystal. In this study, we use ultra-high resolution aberration-corrected electron microscopy to probe the underlying atomic scale chemistry and physics that can tailor the resulting electronic properties of the h-BN. We probe the sub-Ångstrom structural distortions that occur at the defects and edges in h-BN membrane using phase contrast imaging, scanning transmission electron microscopy and electron energy loss spectroscopy.

A bilayer of h-BN is studied in this investigation. Our experimental investigation along with first-principles calculations show formation of interlayer bonds across the bilayer h-BN membrane, leading to symmetry breaking at the boron monovacancies and at the edges [4]. This structural distortion alters the scattering potential, further leading to a significant phase shift around the boron monovacancies and edges (Fig. 1). Such a phase shift leads to the chemical identification of boron monovacancies as opposed to nitrogen defects due to the fact that the latter do not form interlayer bonds leading to phase shift.

We observe formation of large terraces and step edges across the h-BN as a result of sample beam interactions. These edges are mostly formed along the zigzag direction. Similar to monovacancies, atomic column EELS analysis and Z contrast imaging coupled with *ab initio* calculations reveal interlayer B-N bond formation across the zigzag edges in h-BN (Fig. 2). Such interlayer bonds are observed along the zigzag edges and give rise to a higher intensity in Z contrast ADF images due to different electron beam channeling at the distorted edges. Our density functional theory calculations show that such atomic relaxations in h-BN can significantly alter the electronic properties of this crystal.

Such distortions are at the heart of the condensed matter physics and can significantly alter the chemical, physical and electronic properties of h-BN.

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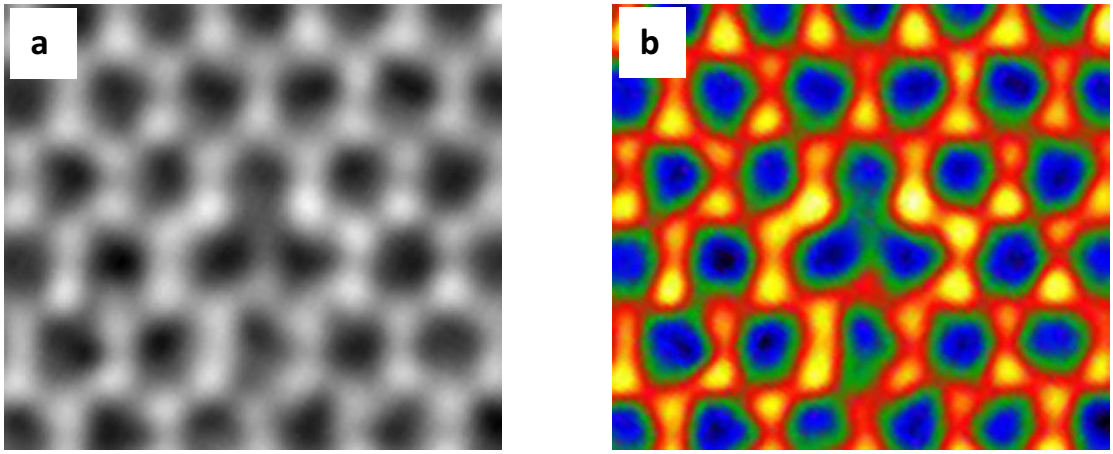

Fig 1. A boron monovacancy (a) with its false color image (b) in a bilayer h-BN showing an assymetry in the in-plain view of the vacancy. The false color image shows the atoms at the perimeter of the vacancy with an intesity higher than the background.

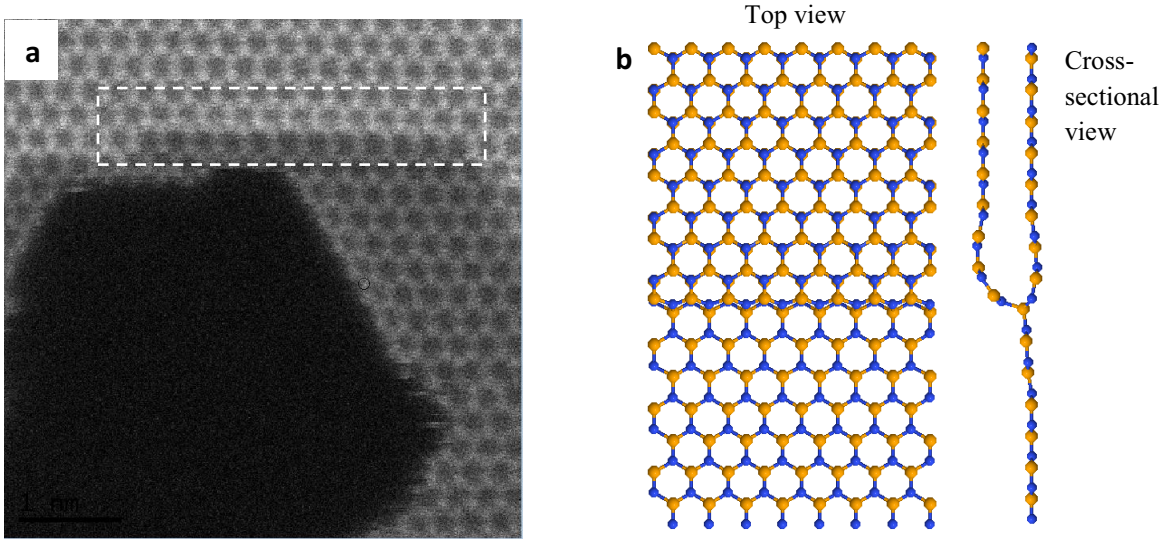

Fig 2. An annular dark field STEM image of a bilayer h-BN (a), showing step edges with zigzag configuration in the assigned region. Density functional theory calculations predict interlayer bonds at the edges of h-BN leading to the distortion of the film (b).