The Atomic and Electronic Structure of Phosphorene

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Abstract

Black phosphorus or phosphorene received considerable scientific interest over half a century ago due to its unusual stability compared to other phosphorus allotropes as a result of its unique crystal and electronic structure[1]. The recent emergence in 2-dimensional materials, however, has led to a rediscovery of phosphorene as a layered 2D material with considerable applicability[2]. While first principle studies have predicted both the atomic and electronic structure of phosphorene, atomic resolution experimental evidence to support the theoretical predictions would verify and further our understanding of this material. In this work, scanning transmission electron microscopy (STEM) was used to image few-layer phosphorene with atomic resolution to provide directly interpretable images of its crystal structure in three different zone axes models of which are shown in Figure 1. The experimentally measured lattice parameters match those predicted by simulation[4]. In addition, low-loss and core-loss electron energy loss spectroscopy (EELS) were used to analyze the electronic structure of this material. The resulting conduction band density of states measurements closely resembled those from DFT calculations. The effects of oxidation of phosphorene were also explored using a STEM-EELS approach which explained the degradation observed in devices.

References

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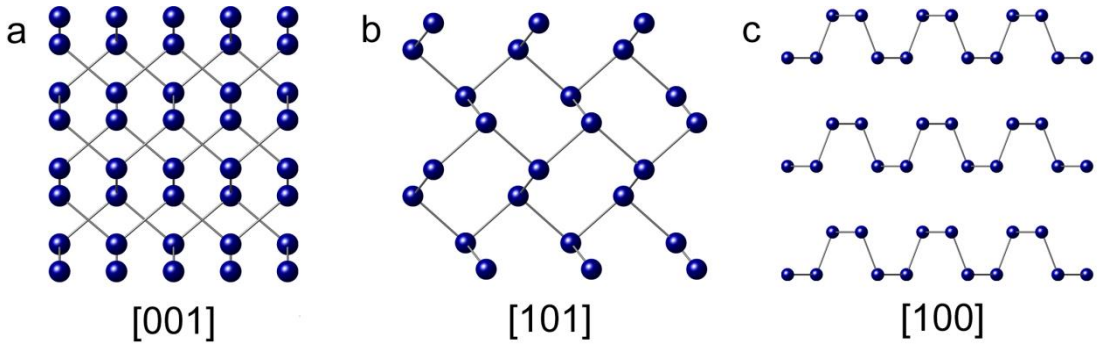

Figure 1: Structure of Black Phosphorus. **a)** top down view or [001] zone axis. **b)** 17.5 degrees off of [001] or [101] zone axis. **c)** cross sectional view or [100] zone axis.