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Electronic Bandgap and Edge Reconstruction in Phosphorene: An Experimental/Theoretical joint investigation[1] LIANGBO LIANG, Rensselaer Polytech Inst, JUN WANG, WENZHI LIN, BOBBY G. SUMPTER, MINGHU PAN, Oak Ridge National Laboratory, VINCENT MEUNIER, Rensselaer Polytech Inst — Phosphorene, or monolayer black phosphorus, is a new 2D layered material with high hole mobility and direct semiconducting bandgap. However, the direct bandgap of phosphorene has not been directly measured, and the properties of its edges have not been considered in detail. In a joint experimental/theoretical work, we studied the electronic properties of phosphorene and its edges [Liang et al., Nano Letters, 2014, 14, 6400]. A detailed scanning tunneling microscopy/spectroscopy (STM/S) study with first-principles calculations reveals the presence of a semiconducting 2 eV gap, the direct bandgap for phosphorene. More importantly, we were able to identify a sharp mono-step in phosphorene that allowed us to perform the first-ever investigation of edges. STS measurements across the step edge indicate nontrivial multiple edge states located inside the 2 eV gap and below the Fermi level. To understand these edge states, we have modeled a series of 1D phosphorene nanoribbons including armchair- and zigzag-edged PNRs. Extensive density functional theory calculations show that edge reconstructions are responsible for energy positions of these edge states. The reconstructions self-passivate most edge dangling bonds by switching the coordination number of phosphorus from 3 to 4 or 5.

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