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Quasiparticle Band Gap and Band Gap Reduction of Multi-Layer Black Phosphorus in an External Electric Field VY TRAN, LI YANG, Washington University in St Louis — Few-layer black phosphorus has emerged as a promising 2D semiconductor due to its highly tunable, direct band gap. In this talk, we examine the tunability of the band gap with respect to the number of layers and the under an external electric field. Using the results of DFT as well as many-body GW calculations, we explore the mechanism for the band gap reduction when increasing the number of layers in black phosphorus. We propose a simple model that describes this behavior, allowing us to calculate the band gap of multi-layer black phosphorus under an external electric field. The results are checked against *ab-initio* calculations, which shows excellent agreement. This allows us to overcome the limitations of DFT and predict the band gap for much larger layer numbers and electric field strength.

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