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Encapsulation-induced Renormalization of the Electronic and Optical Bandgaps in Black Phosphorene Nanostructures DIANA Y. QIU, FELIPE H. DA JORNADA, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — Few-layer black phosphorus has recently emerged as a promising 2D semiconductor, notable for its widely tunable bandgap, highly anisotropic properties, and theoretically-predicted large exciton binding energies. In order to avoid degradation under ambient conditions, it has become common practice to encapsulate black phosphorus devices, and it is generally assumed that this encapsulation does not significantly affect their electronic and optical properties. We have performed ab-initio GW and GW plus Bethe Salpeter equation (GW-BSE) calculations to determine the quasiparticle (QP) bandstructure and optical spectrum of one (1L)- through four-layer (4L) black phosphorus, with and without encapsulation between hexagonal boron nitride and sapphire, two of the most common capping and substrate materials. We find that due to its small intrinsic screening, black phosphorus is exceptionally sensitive to environmental screening. Encapsulation reduces the exciton binding energy in 1L by as much as 70% and completely eliminates the presence of a bound exciton in 4L. The reduction in the exciton binding energies is offset by a similar renormalization of the QP bandgap so that the optical gap remains unchanged, though the qualitative features of the absorption spectrum change dramatically.

Diana Y. Qiu
University of California at Berkeley and Lawrence Berkeley National Lab

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