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GW-Bethe-Salpeter study of the optical properties of graphane¹ HOONKYUNG LEE, MARVIN L. COHEN, STEVEN G. LOUIE, Department of Physics, University of California, Berkeley. Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California, BERKELEY TEAM — Recently, hydrogenated graphene (i.e., graphane) has been synthesized experimentally. Interesting properties such as reversible hydrogenation and transforming from a metal into an insulator have been observed. According to a recent study [Lebegue et. al., Phys. Rev. B 79, 245117 (2009)], the band gap of graphene is open up from 0 to ~5 eV through the hydrogenation of graphene to graphane. In this talk, we will present results of a first-principles study of the optical properties of graphane using the GW-Bethe-Salpeter equation approach.

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