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Quasiparticle Band Gap modulation in Graphene Nanoribbons Supported on Weakly interacting Surfaces XUEPING JIANG, Rensselaer Polytechnic Institute, NEERAV KHARCHE, Brookhaven National Laboratory, PAUL KOHL, Georgia Institute of Technology, TIMOTHY BOYKIN, The University of Alabama in Huntsville, GERHARD KLIMECK, Purdue University, MATHIEU LUISIER, Integrated Systems Laboratory,, PULICKEL AJAYAN, Rice University, SAROJ NAYAK, Rensselaer Polytechnic Institute — Low dimensional nanostructures such as graphene nanoribbons(GNRs) and hexagonal boron nitride (hBN) have been successfully synthesized in experiments and attract a lot of attention recently. The strong electron-electron interactions due to quantum confinement could alter band gaps of nanostructures, which has been studied thoroughly for GNRs. Band gaps could also be changed by the effect of dielectric screening arising from the surrounding materials such as the substrate. However, this effect has not been thoroughly investigated for GNRs. In contrast, in almost all the experiments GNRs are deposited on different dielectric substrates leaving a gap between theoretical estimates and experimental measurements. The effect of dielectric screening cannot be captured in an effective single particle theory such as the density functional theory (DFT) and the many-body approaches such as GW are required. We show the band gaps of the free standing GNRs are reduced as much as 1 eV in spite of weak van der Waals interactions between the GNR and the underlying substrate. This non-local effect can be explained by a semi-classical image charge model and such understanding is critical to the band gap engineering of graphene based devices.

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