Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Substrate Screening Induced Renormalization of Excited-States in 2D Materials NEERAV KHARCHE, VINCENT MEUNIER, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, NY 12180 — Two-dimensional (2D) materials offer an emerging platform for exploring novel electronic phenomena in reduced dimensionality systems. However, because of their atomic scale thickness, their excitation energy levels in 2D materials are strongly renormalized due to the screening by the surrounding environment. This effect is expected to have strong impact when the materials are integrated into functional devices. For example, the presently available GW calculations significantly overestimate the band gaps in graphene nanoribbons (GNRs) by as much as one eV compared to experiment. Here, we outline an integrated computational approach combining DFT, the GW approximation, and a classical image charge model to include substrate screening effects in a computationally tractable manner. We investigate the band gaps and defect charge transition levels (CTLs) in a prototypical 2D material, hexagonal boron nitride (hBN) and a prototypical 1D nanostructure, GNR. The band gaps and defect CTLs are strongly renormalized by several tenths of an eV in the substrate-supported versus the free-standing configurations. In the case of GNRs, the predicted band gaps are in an excellent agreement with recent STS experiments.

Neerav Kharche
Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, NY 12180

Date submitted: 05 Nov 2015 Electronic form version 1.4