**Substrate Screening Induced Renormalization of Excited-States in 2D Materials**

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**Abstract**

Two-dimensional (2D) materials offer an emerging platform for exploring novel electronic phenomena in reduced dimensionality systems. Owing to their atomic scale thickness, the excitation energy levels in 2D materials are strongly renormalized due to the screening by the surrounding environment such as the substrate. This effect is expected to have strong impact when the 2D materials are integrated into functional devices. Accounting for such long-range screening requires methods beyond density functional theory (DFT), such as the GW approach. Large scale GW calculations including the substrate are not feasible using the presently available computational tools.

We have developed an integrated first-principles approach combining density functional theory (DFT), the GW approximation, and a semiclassical image-charge model to compute the electronic band gaps in planar 2D systems in weak interaction with the surrounding environment, including long-range screening effects, in a computationally tractable manner.[1] This methodology is general for any planar 2D system and we apply it here to the specific case of graphene nanoribbons (GNRs) since accurate experimental data exist.[2,3]

We find that the band gap of substrate-supported GNRs is reduced by several tenths of an eV compared to their isolated counterparts, with a width-and orientation-dependent renormalization. The predicted band gaps are in good agreement with the range of available experimental data on substrate-supported armchair GNRs (Figure 1). Our results indicate that the band gaps in GNRs can be tuned by controlling the electronic screening at the interface and suggest the interesting possibility of using spatially varying dielectric environment to engineer the screening effects and induce band offsets into 2D materials without any chemical modification.

**References**

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**Figures**

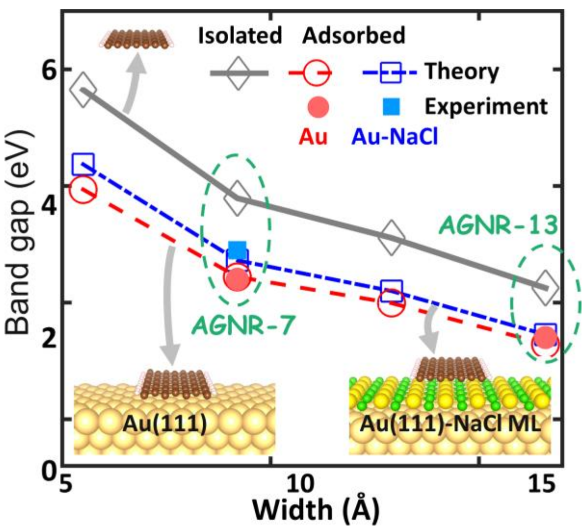


**Figure 1:** Quasiparticle band gap of the isolated and substrate-supported armchair graphene nanoribbons (AGNRs) as a function of their width. Energy levels in the substrate supported AGNRs are strongly renormalized by the substrate induced screening effect resulting in the reduction of the band gap.