Phosphorene: Graphene's Difficult Cousin

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Abstract:

From all the two-dimensional materials discovered after graphene, phosphorene holds a special place due to the fact that it is composed of a single atom type. Its corrugated structure gives rise to a highly anisotropic dispersion and the presence of a gap makes it an appealing candidate for potential applications. The size of the gap can be modified by applying uniaxial strain, which can potentially even lead to the closing of the gap. Unfortunately, unlike graphene, which can be modeled using the tight binding model, phosphorene's bands cannot be described using a simple nearest-neighbor approximation. As a consequence, one typically has to resort to *ab initio* calculations. Using the first principles calculations, we study nanoribbons in phosphorene and show that depending on the edge type, the ribbons can give rise to localized edge states. While the analytical treatment of the problem is non-trivial, it is possible to make some definite predictions for one of the edge types.

Having obtained the band structure using numerical methods, we address the issue of excitons in anisotropic two-dimensional systems. Employing a combination of analytical and numerical methods, we obtain the binding energies for excitons and show how they change with the substrate and applied strain. Our results compare favorably with those reported earlier using different approaches. Additionally, we study the dynamic polarization in monolayer and double-layer phosphorene. We show that double-layer systems give rise to two distinct plasmonic branches, as was previously reported for graphene. Here, however, the system anisotropy introduces additional effects, such as anisotropic Landau damping and effective gating due to relative twist between the layers.

References:

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