Two-dimensional nitrides for ultraviolet to infrared detectors

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Group-III Nitrides have received great attention for high-power electronic devices and for optoelectronic applications such as light-emitting diodes. In addition, in recent years, theoretical and experimental studies on graphene have provided a wide range of knowledge for a new class of 2D materials. Motivated by these recent developments, we present here a systematic ab-initio study of the electronic and optical properties of two-dimensional Nitrides (BN, AlN, GaN, InN, TlN). In particular, the geometry is investigated within Density Functional Theory, while the electronic and optical properties are calculated with the Many Body Perturbation Theory in the GW approximation and by solving the two-particle Bethe Salpeter equation.

2D-Nitrides are predicted to have a honeycomb flat structure like graphene. Our results show that with increasing group-III atomic number, a decrease of the gap from 6.7 eV to a few meV takes place. Interestingly, 2D GaN and InN present a direct gap at Γ. For what concerns the optical properties, we have investigated the excitonic behavior of this class of materials using the Bethe Salpeter Equation and a simple analytical model for 2D systems. Our results demonstrate that 2D Nitrides sheets possess strongly bound excitons due to the interplay of low dimensionality, depressed screening and the presence of a gap. By exploiting the reduced dimensionality and the chemical trend, we show that it is possible to engineer their electronic and optical response, and suggest that the emission range of optoelectronic devices based on 2D group-III Nitrides varies from UV to visible. Additionally, with the goal of tailoring devices properties by taking advantage of the characteristics of individual materials, we have studied 2D-Nitrides alloys and heterostructures. Band alignments calculations suggest a that BN/AlN form a type I heterostucture. By alloying GaN , TlN and InN we show that it is possible to tune the gap from UV to IR and form type II alignment. Sandwiched graphene and BN layers are also investigated.

These novel heterostructures based on the vertical stacking of different hexagonal 2D crystals may be important for light harvesting and photovoltaic applications.