Excitonic complexes in anisotropic few-layer two-dimensional materials

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Among the vast variety of recently discovered two-dimensional (2D) layered materials, phosphorene has attracted particular interest, due to its unique properties, namely a direct band gap with a highly anisotropic band structure and high carrier mobilities. [1] The (still theoretical) few-layer arsenic [2] and other layered materials in the chalcogenides family, such as ReS2 and TiS3 [3], have also been recently demonstrated to exhibit band anisotropy. This feature gives rise to unique physical properties, e.g. direction-dependent effective masses, mobilities, and excitonic polarizabilities, features expected to enable avenues for new device applications.

Interest in excitonic complexes in phosphorene has recently been boosted by experimental claims of trion binding energies as high as ~ 100 meV, as a consequence of the band anisotropy. [4] Such a huge trion binding energy would be of great importance, allowing for possibly driving the trion by in plane electric fields without dissociation. It is then particularly interesting to theoretically verify this trion energy not only in phosphorene, but also in other anisotropic 2D materials.

In this work, excitons, trions and biexcitons in anisotropic two-dimensional materials are investigated within an effective mass theory. Explicit results are obtained for phosphorene, arsenene, and TiS3. Theoretical results for excitons in few-layer phosphorene are shown to be in very good agreement with experimental ones, see Fig. 1. Trions are predicted to have remarkably high binding energies and an elongated electron-hole structure with a preference for alignment along the armchair direction, where the effective masses are lower. Biexciton binding energies are also notably large, especially for monolayer phosphorene, where they are found to be twice as large as those for typical monolayer transition metal dichalcogenides.

References

Figures

Figure 1: Ground state (inset) and separation between 1s and 2s states as a function of the number of phosphorene layers. Experimental and theoretical results are compared [5].