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Two-dminensional exciton states in monolayer semiconducting phosphorus alotropes[1] ALEXANDRE R ROCHA, CESAR E P VILLEGAS, Instituto de Fisica Teorica - Unesp, Sao Paulo, Brazil — During the last decade, novel two-dimensional (2D) semiconducting materials have been synthesized and characterised. As a result, there have been several theoretical and experimental proposals to incorporate 2D materials for designing next generation electronic and optoelectronics devices. In particular, it has been demonstrated that light absorption in phosphorus-based monolayers can span the whole visible spectrum, suggesting they could be used for optolectronic applications. A key ingredient for optolectronic applications is the presence of excitons and their subsequent diffusion along a donor material. This is influenced by the character of the different excitations taking place, as well as, the exciton binding energy. Therefore, In this work we use accurate many-body corrected density functional theory by means of GW-BSE methodology to elucidate the most important optical transitions, exciton energy spectrum as well as exciton extension in different types of phosphorene materials. In addition, we solve the Schrodinger equation for different 2D screened potentials and estimate the 2D exciton energy levels and radius extension. Finally, in order to assess further studies based on these systems, we provide a simple analityc expression for estimating 2D exciton energy levels.

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