Excitonic effects in novel 2D materials and vdW heterostructures

Since the first successful exfoliation of graphene (a monolayer of graphite), the family of two-dimensional (2D) materials has grown tremendously and will continue to grow in the future. Typical 2D materials, represented by monolayers of graphite, black phosphorus, and transition metal dichalcogenides, have exceptional electronic and optical properties such as high carrier mobility and strong optical absorption, which make them very promising for electronic and optoelectronic applications. By combining different 2D materials vertically or laterally, vertical or lateral van der Waals (vdW) heterostructures can be formed. To date, a lot of vdW heterostructures have been prepared and designed to improve the properties of single 2D materials. The formation of vdW heterostructures makes 2D materials have greater advantages over traditional 3D materials in realizing new functions. Compared to 3D materials, 2D materials and vdW heterostructures feature strong quantum confinement and reduced dielectric screening, leading to enhanced fascinating many-body effects induced by carrier-carrier interaction and correlation. One of the most prominent examples is high-temperature exciton condensation and superfluidity realized in vdW heterostructures [1, 2]. In order to understand deeply such correlated many-body states, it is very essential to explore the primary driving force behind them, i.e., excitonic effects. Such many-body effects dominate not only the properties of light absorption but also the dynamics of photo-generated carriers in 2D materials and vdW heterostructures. Here, using state-of-the-art theoretical and computational approaches based on density-functional theory and many-body perturbation theory, we will investigate optically anisotropic excitons (both interlayer and intralyer excitons and their binding energies, oscillator strengths and wave functions) and how they can be tuned by mechanical strain and electrical gating in vdW heterostructures of black phosphorus and arsenide. Our theoretical investigation is expected to provide reliable and accurate insights into designing 2D novel excitonic devices using anisotropic vdW heterostructures.

References

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