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【507】 Characterization of Excitons for bulk Black Phosphorus

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Excitons (coupled electron–hole pairs) in semiconductors can form collective states that exhibit spectacular nonlinear properties and possible applications in future optoelectronic devices.

We present here some theoretical methods and a workflow for determining the excitonic wave functions and the corresponding excitonic binding energies for bulk Black Phosphorus. We solve the Bethe-Salpeter equations for coherent and incoherent excitations. The theoretical/numerical results are compared to the experimental ones of angle resolved photoemission spectroscopy (ARPES) to understand the nature and characteristics of these two-particle bound states, being challenging due to the stronger screened potential for 3D materials, resulting in short time excitations.

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