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Anisotropic Exciton Properties of Phosphorene

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Abstract

Phosphorene, a two-dimensional (2D) material with strong in-plane anisotropy, exhibits unique excitonic behavior. In this work, we investigate the anisotropic optical and dynamical properties of excitons in phosphorene by combining microscopic many-body theory with first-principles calculations. Our workflow combines previous approaches, offering a complete and material specific description of the excitonic properties of phosphorene. We compute exciton states and optical absorption spectra, revealing direction-dependent characteristics. Furthermore, we study exciton relaxation dynamics and transport, highlighting the critical role of long-range exchange interactions. Notably, we find that these interactions significantly enhance the anisotropy of exciton diffusion, particularly at low temperatures. Our findings provide a recipe for the design of excitonic circuits for highly controllable energy transport in optoelectronic devices.