

Optical and Excitonic Properties in 2D Materials and van der Waals Heterostructures Using Many-Body Methods

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Electron-electron and electron-hole (exciton) effects are specifically pronounced in two-dimensional (2D) materials because of weak dielectric screening from the environment. We review here our achievements in the field in the last several years. We recently showed strong effects of excitons on optical absorption in functionalized graphenes [1-2], III-V and V-V hexagonal semiconductors [3-4], or transition metal carbides (MXenes) [5-8], resulting also in the excitonic insulator phenomenon [9]. Besides accurate Bethe-Salpeter equation calculations, we also proved that time-dependent density functional theory (TD-DFT) based on specific screened hybrid density functional can effectively account for all important physical effects, including excitons [10-11], thus, it is a practicable technique for van der Waals heterostructures containing incommensurate cells of different monolayers [12].

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Figures

