Excitons in Two-Dimensional Materials

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Two-dimensional van der Waals materials exhibit novel photoexcited states, intriguing field-driven and time-dependent phenomena, and exotic ground states. Here, we present some recent theoretical advances in their understanding and predictions. Our studies reveal a rich diversity of excitons in transition metal dichalcogenide (TMD) moiré superlattices, including previously unforeseen intralayer charge-transfer moiré excitons. We have also discovered a self-driven exciton-Floquet effect in the time-resolved, angle-resolved photoemission spectroscopy of 2D materials, where exciton-induced satellite features and band renormalization emerge, analogous to the optical Floquet effect driven by photons. We further show that strong excitonic physics in 2D materials can greatly enhance their nonlinear optical responses, such as shift currents and second- or higher-order harmonic generation. This has led to the discovery of a remarkable phenomenon – the formation of light-induced shift current vortex crystals in TMD moiré systems. Finally, we predict that in certain intrinsic TMD 2D materials, spontaneously formed excitons condense into an unconventional excitonic insulator phase, characterized by emergent **k**-space spin textures and other telltale spectroscopic signatures. This work was supported by the U.S. Department of Energy and National Science Foundation.