Laterally Extended States of Interlayer Excitons in Reconstructed MoSe₂/WSe₂ Heterostructures

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Heterostructures made from 2D transition-metal dichalcogenides are ideal platforms for exploring excitonic phenomena, including correlated moiré excitons and degenerate interlayer exciton ensembles. While atomic reconstruction is often assumed to localize excitons, we demonstrate that excitonic states in reconstructed MoSe₂/WSe₂ heterostructures can extend beyond the moiré periodicity [1]. Using real-space calculations, we provide lateral potential maps and corresponding excitonic wavefunctions for interlayer excitons in strain-relaxed heterostructures [2]. Cryogenic photoluminescence experiments support the computed level structure and exciton relaxation dynamics. These findings align with recent coherence measurements on degenerate interlayer excitons and suggest potential many-body phenomena in dense, cold exciton ensembles [3].

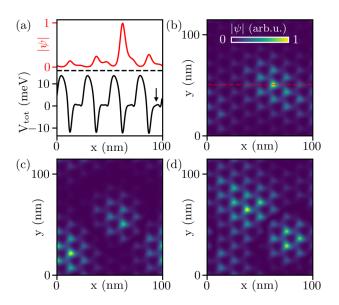


Figure 1: (a) Top curve: Absolute value of the center-of-mass (COM) wavefunction Ψ for the first interlayer exciton (IX) eigenstate along the crystallographic direction of a reconstructed bilayer at 1.3° twist angle. Bottom curve: Corresponding total IX potential along the same direction. The arrow indicates one of many small variations of V_{tot} caused by the introduced imperfections within the simulated sample. (b-d) The absolute value of the COM wavefunction of the first three IX eigenstates in real space.

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References

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