Modulating Charge-Transfer Doping and Lateral Heterojunctions in $MoSe_2$ Monolayers via Epitaxial High-k Dielectric Thin Films

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Layered transition metal dichalcogenides (TMDCs) have become a central focus in 2D materials research due to their exceptional properties at the monolayer (ML) level. For practical applications, integrating these materials with suitable dielectrics is crucial. The excitonic and electronic properties of 2D TMDCs are highly sensitive to their dielectric environment, offering unique opportunities for interface engineering. As a case study, I shall discuss the influence of epitaxial high-k Gd_2O_3 thin films on the excitonic emission from $MoSe_2$ MLs. Our research demonstrates that integrating two differently oriented epitaxial Gd_2O_3 layers significantly enhances trion emission, with a two-fold increase in trion intensity for $MoSe_2$ on Gd_2O_3 (110) compared to Gd_2O_3 (111). This enhancement is attributed to surface charge transfer doping of the $MoSe_2$ MLs, controlled by the epitaxial orientation of the Gd_2O_3 layers. Detailed studies revealed a higher concentration of oxygen vacancies on the Gd_2O_3(110) surface compared to the Gd_2O_3(111) surface, due to surface termination-dependent formation energies of the oxygen vacancies. We further demonstrate a lateral dielectric heterojunction within a single $MoSe_2$ ML bridging low-k hBN and high-k Gd_2O_3, forming a spontaneous type-I n^+/n junction without chemical modification. The resulting blue-shifted excitonic features reflect bandgap renormalisation and local charge redistribution driven by dielectric contrast

These results demonstrate the potential of epitaxial dielectrics as tunable platforms for controlled excitonic and electronic modulation in 2D semiconductors.

References

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