Engineering Band Structure Transitions in WSe_2 through Te Doping: An Alternative Approach Beyond Thickness Reduction

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Transition metal dichalcogenides (TMDs) hold significant promise for next-generation electronics applications, particularly as their thickness is reduced to several atomic layers, leading to dramatic changes in their electrical and optical properties. For instance, TMDs such as MoS_2, $MoSe_2$, WS_2, and WSe_2 exhibit a transition from an indirect to a direct band gap when reduced to monolayer thickness. Leveraging these unique and diverse properties, TMD materials show great potential for future electronic devices. In this study, we propose an alternative method to induce a transition from an indirect to a direct band gap in WSe_2 by slightly doping Te atoms. WSe_2 single crystals with varying Te content were synthesized using the floating zone method, with the Te doping level calibrated by x-ray photoemission spectroscopy (XPS). Through angle-resolved photoemission spectroscopy (ARPES) and density functional theory (DFT) calculations, we investigate the evolution of the band structure of slightly Te-doped WSe_2. With increasing Te content, we observe a shift of the valence band maximum from the Γ point to the K point. DFT calculations reveal that the conduction band minimum remains at the K point, indicating a transition from an indirect to a direct band gap due to Te doping. Our work presents an alternative approach to engineering the band structure of WSe_2, distinct from thickness reduction.