Exploring Dopant-Defect Interactions and their Impact on Optoelectronic Properties in Vanadium-Doped WS_2 Monolayers

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Transition Metal Dichalcogenides (TMDs) such as WS_2 have garnered considerable attention as promising candidates for next-generation transistor, sensor, and quantum photonic devices due to their favorable optoelectronic properties. Substitutional doping (controllably replacing an intrinsic atom with a foreign atom) is widely used to tune the optical, electronic, and magnetic properties, in two dimensional TMDs. Despite the promise of substitutional doping, the underlying interactions between dopants and intrinsic defects within TMDs is an area of open research. This study reports the intricate interplay between doping and defect engineering in vanadium doped WS_2 monolayers synthesized via Atmospheric Pressure Chemical Vapor Deposition (APCVD). By systematically analyzing the effects of vanadium doping on the photoluminescence (PL) properties, structural characteristics, and electronic transitions of WS_2 monolayers, we uncover how dopant-defect interactions modulate the electronic structure and optoelectronic properties within this class of material. Particularly, our findings reveal that doping WS_2 with low (< 0.2 atom%) concentrations of vanadium reducing negative trion contributions and enhance PL from the WS_2. Conversely, dopant-defect complexes at higher (> 0.2 atom%) vanadium concentrations introduce deep in-gap states that quench PL by accelerating Auger recombination within the material. These results offer avenues for nanoengineering tungsten disulfide's functional properties, potentially benefiting applications in catalysis, single-photon emission, and beyond.