Engineering Defect States via Oxygen Passivation in Monolayer $MoSe_2$ for Enhanced Photodetection

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Heterostructure-based photodetectors often suffer from limited performance due to strong interlayer coupling and constrained band modulation.[1] As an alternative, defect and doping engineering in 2D transition metal dichalcogenides (TMDs), particularly via hole doping, offers an effective route to tailor their electronic and optoelectronic properties. Here, we demonstrate oxygen passivation of selenium vacancies in monolayer $MoSe_2$ (O_P-$MoSe_2$) and systematically compare it with vacancy-rich $MoSe_2$ (V_{Se}-$MoSe_2$) in terms of structural, chemical, and optoelectronic characteristics, highlighting its applicability for weak-light photodetection. Raman, photoluminescence, and X-ray photoelectron spectroscopy confirm enhanced structural integrity and optical quality upon oxygen passivation. Low-temperature PL measurements reveal suppressed inhomogeneous broadening and the emergence of biexcitonic features, indicating modified excitonic interactions. First-principles calculations show that oxygen preferentially occupies selenium vacancy sites, effectively passivating defect-induced states.[2] As a result, O_P-$MoSe_2$ photodetectors exhibit exceptional performance under 530 nm illumination, achieving a responsivity of 0.74×10^5 A W^{-1}, a detectivity of $\sim 10^{14}$ Jones at 89 nW cm^{-2}, and a low noise-equivalent power of 0.087 fW $Hz^{-1/2}$. Furthermore, the devices enable weak-light tracking of moving objects at different speeds, emulating practical security surveillance scenarios. These results establish oxygen-passivated $MoSe_2$ as a viable platform for ultra-sensitive, low-light photodetection and underscore oxygen passivation as an effective defect-engineering strategy compared to other 2D photodetectors.[3][4]

References

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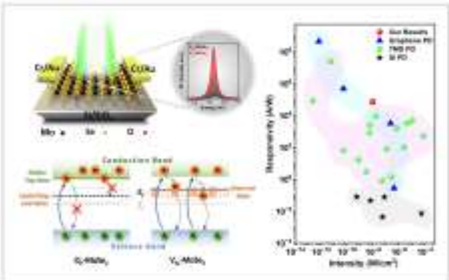

Figure 1: Graphical abstract.