Defect Engineering in 2D MoS_2: Tailoring Optical Properties via Electron Beam Irradiation

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Monolayer molybdenum disulfide (MoS_2) has emerged as a promising two-dimensional (2D) material due to its exceptional optical and electronic properties, making it ideal for applications in electronics, optoelectronics, and quantum technologies. In the 2D regime, quantum confinement effects reduce dielectric screening, thereby enhancing excitonic binding energy and providing an optimal platform for exploring light-matter interactions. However, defects such as point defects, line defects, adatoms, and grain boundaries strongly influence device performance by altering carrier concentration, scattering pathways, mobility, and light emission characteristics [1,2]. Owing to the large surface-to-volume ratio, the structural characteristics of MoS_2 can be easily modulated through extrinsic means. Herein, we employ a high-energy electron beam to induce defects in CVD-grown monolayer MoS_2, enabling the tuning of its structural and optical properties. Room temperature Raman spectroscopy revealed noticeable shifts in prominent E_{2g}^1 and A_{1g} peak positions after irradiation, whereas photoluminescence spectra showed significant quenching. Low-temperature photoluminescence spectra exhibited a broad defect-activated luminescence peak approximately 0.2 eV below the excitonic transition. The spectral weight of defect-bound emission was significantly higher in electron beam-irradiated samples. Additionally, valley polarization was found to be negligible in electron beam-irradiated MoS_2. X-ray photoelectron spectroscopy and kelvin probe force microscopy further confirmed irradiation-induced defects in monolayer MoS_2. Our study highlights the potential of high-energy electron beam irradiation for defect engineering in 2D-MoS_2, paving a way for tailoring its electronic and optical properties.

References

[1] Chow, Philippe K., et al. "Defect-induced photoluminescence in monolayer semiconducting transition metal dichalcogenides." *ACS nano* 9.2 (2015): 1520-1527.
[2] Hou, Chao, et al. "Photoluminescence of monolayer MoS2 modulated by water/O 2/laser irradiation." *Physical Chemistry Chemical Physics* 23.43 (2021): 24579-24588

Figures

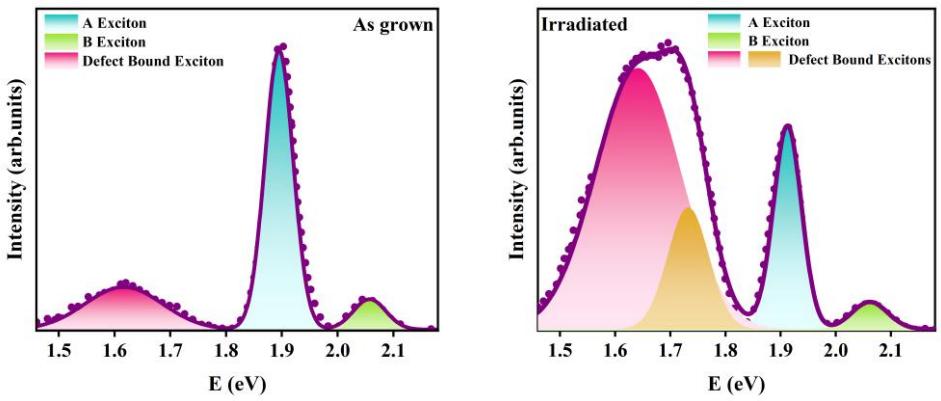

Figure 1: Photoluminescence Spectra of monolayer MoS_2 at 85K before and after electron beam irradiation.