

Theoretical Evaluation of TMDCs as Photosensitizers:

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Abstract

This project analyzes the potential of TMDCs as photosensitizers for opto-biomedical applications. Key concepts are first clarified, and the topic is framed within the context of the Sustainable Development Goals. The scientific background highlights the outstanding optoelectronic properties of 2D materials while pointing out, based on current literature, limitations such as underestimated electronic band gaps, lack of spin-orbit corrections, and incomplete excitonic analyses. The influence of electronic structure and excitonic properties is examined, emphasizing the photosensitization efficiency of MoSe_2 and WSe_2 monolayers. A rigorous computational approach is outlined, following the path from literature insights to experimental validation, providing a reliable and comprehensive assessment of the photosensitizing capabilities of these promising 2D materials.

Keywords: Theoretical modeling, TMDCs, Photosensitizers, Excitons