Theoretical Evaluation of TMDCs as Photosensitizers

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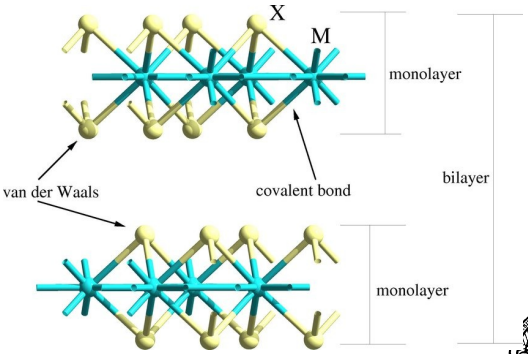
Outline

Definition and Explanation of Keywords

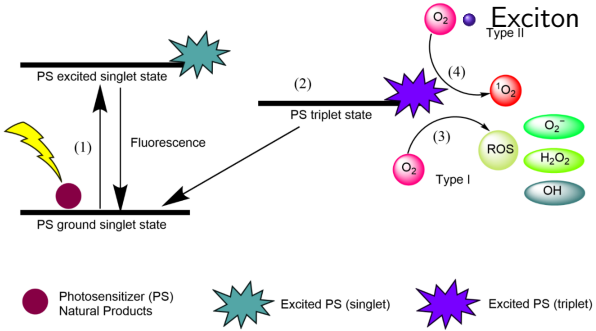
- **Theoretical evaluation: DFT, TD-DFT**

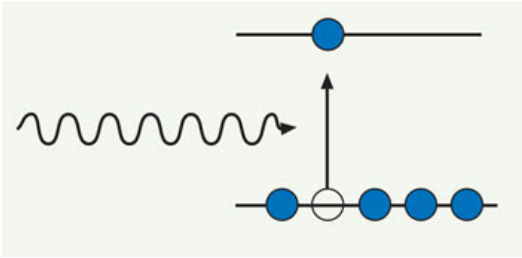
- TMDCs (Transition Metal Dichalcogenides)



Definition and Explanation of Keywords

- Photosensitizer





Subject Reformulation

Research Focus

Theoretical evaluation of the electronic and optical properties of TMDC monolayers (e.g., $MoSe_2$ and WSe_2) using advanced methods (DFT, TD-DFT), to assess their potential as photosensitizers for opto-biomedical applications

Sustainable Development Goals (SDG)

SDG Connection - Potential Links

SDG 3

Good Health and Well-Being

Potential application in photodynamic therapy (PDT) for cancer treatment

SDG 9

Industry, Innovation, and Infrastructure

2D materials research

Advanced computational modeling

Novel optoelectronic technologies

Context

Context

- 2D Materials: emergence of TMDCs ($MoSe_2$, WSe_2)
- Exceptional optoelectronic properties
- Need for efficient photosensitizers for medical applications

Previous work:

- Limited experimental studies on TMDC photosensitizers
- Standard DFT calculations (GGA, LDA)
- Some TD-DFT studies on clusters

Current limitations:

- Underestimation of the gap by standard DFT
- Absence of spin-orbit correction in most studies
- Lack of complete excitonic analysis
- Imprecise optical predictions

Research Problem

Transition Metal Dichalcogenides (TMDCs) like $MoSe_2$ and WSe_2 are promising 2D materials with strong light absorption and pronounced excitonic effects, but their potential as efficient photosensitizers remains unclear. Current experimental data are limited, and theoretical predictions are challenging due to computational approximations, layer-dependent properties, and accurate modeling of excitons and ROS generation

Problematic

Problematic

- How do the electronic structure, excitonic characteristics, and spin-orbit interactions of TMDCs govern their photosensitization efficiency, and how accurately can computational approaches predict their optical and excitonic behavior for effective ROS generation?

Objectives

General Objective

Theoretically evaluate the photosensitizing potential of TMDCs, specifically $MoSe_2$ and WSe_2monolayers, using advanced computational approaches.

Specific Objectives

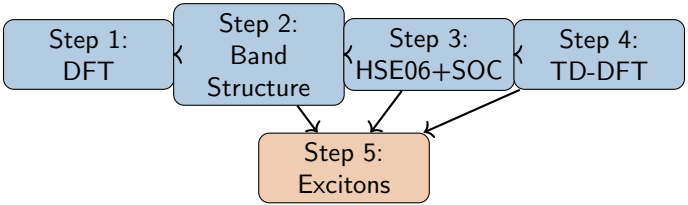
Geometry Optimization and electronic structure determination , with band analysis and density of states (DOS)

Include SOC to capture band splitting near K-point

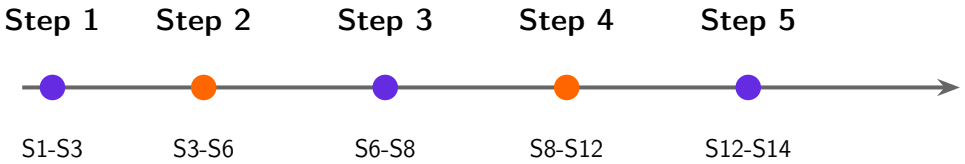
Refine electronic band gap with HSE06

Calculate excited states and analyze electron-hole pair separation efficiency.

Computational Methodology - 5 Steps



Roadmap Timeline



Thank You

For your attention