Master's Thesis Project

Light-Dependent NMR Investigation of Aqueous Carbon Nitride Suspensions

Motivation

Greenhouse gas emissions remain one of the most detrimental anthropological changes that has come about from human existence due to the drastic effects on increasing the temperature of the planet. Fortunately this problem has been previously solved in nature long before humans existed, namely in the form of photosynthesis in plants, whereby carbon dioxide is removed from the atmosphere and stored in sugars and other carbon-rich natural products. Since it was first observed in the 1960s [1], photocatalysis has been at the forefront of scientific discussion with the aim to mimic the harnessing of sunlight and transform this energy into chemical energy available for a number of processes necessary in the industrialized world (Fig 1) [1].

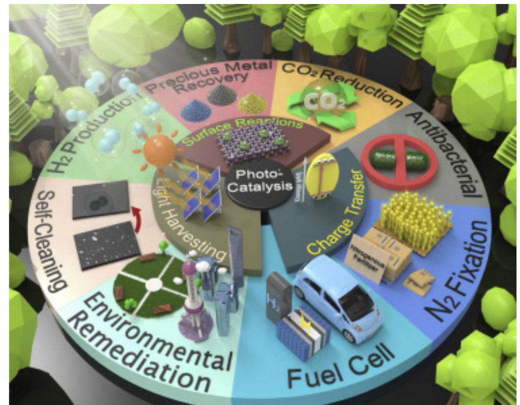

Figure 1: Many of the problems associated with development in the industrialized world may be remedied or solved using photocatalyst materials.

While most photocatalytic materials are composed of or similarly require precious metals and ultraviolet radiation, graphitic carbon nitride (g-C_3N_4) represents one of the most promising metal-free photocatalyst materials available for sustainable chemical processes. Its photocatalytic activity under visible light, instead of UV light, makes it an attractive platform for water purification, CO_2 reduction, and hydrogen evolution [2]. A critical aspect of its performance remains poorly understood: how the surrounding water phase interacts with the carbon-nitride surface. Understanding this interfacial region is essential for improving reaction efficiency and for scaling up laboratory findings to engineered reactors. Nuclear Magnetic Resonance (NMR) offers a unique, non-invasive approach to access this missing information. Through relaxation and diffusion measurements, water dynamics and molecular mobility near the carbon-nitride surface can be resolved with high sensitivity [3]. By introducing controlled in-situ illumination during NMR measurements, it becomes possible to directly monitor how light exposure alters the local water environment, providing a microscopic view of photo-induced processes at the interface [4-5]. This project will therefore focus on the light-dependent NMR investigation of water in carbon-nitride suspensions to establish a mechanistic understanding of how light and surface chemistry jointly control reaction dynamics.

The goal of this project is to investigate the interactions of water on the surface of graphitic carbon nitride particles suspended in aqueous media in both the presence and absence of light irradiation. Investigations of water interactions will be performed using a 60 MHz SpinSolve NMR spectrometer. You will develop knowledge and gain experience in sample preparation, fundamental experimental design, spectroscopic data acquisition methods, and complex data analysis in order to obtain a real-world physical model of your experimental data. Your work will directly contribute to the understanding and optimization of photocatalytic materials for laboratory and pilot scale photoreactors.

Contents of the Work

- Prepare stable aqueous carbon-nitride suspensions.
- Perform ^{1}H-NMR relaxation and diffusion measurements of carbon nitride suspensions under dark and illuminated conditions.
- Quantify illumination-induced changes in relaxation and diffusion parameters.
- Correlate NMR results with carbon nitride surface properties and potential photocatalytic activity.

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Key References

[1] Li et al., *Chem Cat.*, 2022, 2, 1315-1345. [2] Ong et al., *Chem. Rev.*, 2016, 116, 7159-7329. [3] Stankiewicz et al., *J. Phys. Chem. B*, 2024, 128, 1535-1543. [4] Dauth et al., *Angew. Chem. Int. Ed.*, 2024, 63, e202412972. [5] Suekuni et al., *ACS Catal.*, 2025, 15, 2063-2081.