ITI HiFunMat Master Internship Proposal

☐ M 1 ☒ M 2

Solar light driven synthesis of H_2O_2 from H_2O and O_2 on 2D-layered g-C_3N_4 based catalysts

Internship supervisor

Name, first name	KELLER Nicolas
E-mail, Telephone	nkeller@unistra.fr – 03 68 85 28 11 – 06 74 87 52 95
Laboratory	ICPEES UMR 7515 CNRS-Université de Strasbourg
Collaboration with a HiFunMat member (*please indicate their name*)	☒ No ☐ Yes :

Student profile looked for

Master program (*more than one box can be ticked)*	☒ Material science and engineering ☒ Chemistry ☐ Physics
Other indications if necessary	

Internship description

Hydrogen peroxide (H_2O_2) is an efficient and environmentally friendly oxidant due to its large active oxygen content (47 *wt.*%), relatively high oxidation potential (E°=1.763 V *vs.* NHE at pH 0), easy-handling and non-toxic oxidation by-products (water and oxygen). These properties make H_2O_2suitable for varied applications like wastewater treatment (*eg.*, Fenton processes and disinfection), chemical manufacturing or pulp bleaching, with an annual worldwide production over 5 Mt. Moreover, H_2O_2 is also a promising energy-carrier alternative to hydrogen, since it can be used as fuel in single-compartment cells and can be conveniently transported and stored.

Currently, H_2O_2 is produced industrially by the well-known high E-factor and low atom efficiency multi-step anthraquinone process, which requires high energy input and generates large amounts of wastes (*eg.* organics-containing wastewater, solid waste). Thus, it is worth to develop cost-effective and sustainable approaches for H_2O_2 production. In this context, solar light-driven photocatalysis has emerged as it utilizes H_2O and molecular O_2 as raw materials, and solar light as energy supply. Photocatalysis is also a worth strategy for the safe and cost-efficient implementation of decentralized small-scale production units as well as for the *in-situ* synthesis of H_2O_2 for use as oxidant in high-efficiency chemical reactions.

2D-layered graphitic carbon nitride (g-C_3N_4) is a prominent candidate for H_2O_2 synthesis because of its relatively narrow band gap (*ca.* 2.7 eV), suitable electronic structure for O_2 reduction and a high chemical stability [1]. g-C_3N_4 benefits also from easy, low-cost preparation methods, as well as from its metal-free and non-toxic nature.

The internship will study to which extent the photonic efficiency and the production rate of H_2O_2 from H_2O and O_2 under solar light can be significantly enhanced by implementing synthetic strategies based on molecular and electronic modifications of g-C_3N_4 photocatalysts. The work will focus on designing innovative heterogeneous solar-light driven catalysts and their characterizations, as well as on the evaluation of their catalytic behaviors under solar light.

The internship will benefit from the scientific, technical and human resource environment provided by the 'Photocatalysis and Photoconversion' team at ICPEES.

1. *Ru–modified graphitic carbon nitride for the solar light–driven photocatalytic H_2O_2 synthesis,* L. Valenzuela, […], N. Keller **Catal. Today** 441 (2024) 114881 ; *Photocatalysis synthesis of hydrogen peroxide from molecular oxygen and water.* P. Garcia-Munoz, […] N. Keller, **Top. Curr. Chem.** 381(4) (2023) 15