Programa de Doctorat
Eletroquímica. Ciència i Tecnologia

PLA DE RECERCA

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Línia de recerca: Electrochemistry. Science and Technology

Títol de la Tesi: the Electrochemical Conversion of Benzaldehyde and its Device Optimization

El projecte ha de constar de les següents parts:

1. Introducció: interès del tema
2. Objectius
3. Pla de treball i cronograma.
4. Bibliografia

Màxim 1200 paraules (sense comptar la bibliografia)

Introduction

Climate change is one of the greatest threats of our era. a growing world population is increasing the demand for energy. This challenging situation calls for moving away from fossil fuels towards renewable sources of energy and guaranteeing a secure and affordable energy supply globally while protecting the environment[1].

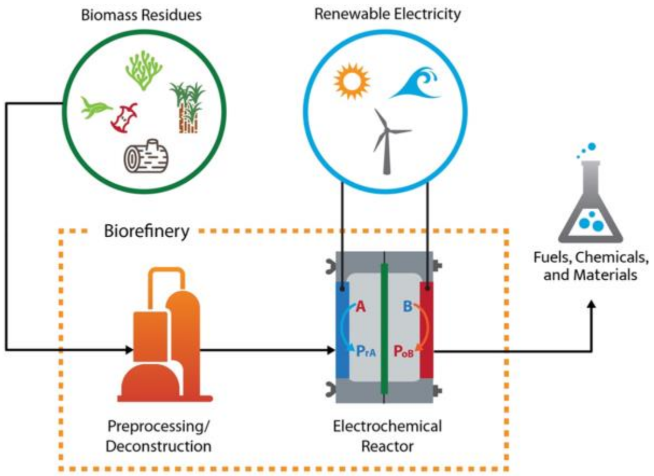

Figure 1. Biorefining with renewable electricity.

Bioenergy will have essential roles in all sectors in the energy transformation and in building a climate-friendly circular carbon economy that delivers economic and social benefits[2]. Modern bioenergy technologies include liquid biofuels produced from bagasse and other plants; bio-refineries; biogas produced through anaerobic digestion of residues; and other technologies (Figure 1). Therefore, researches on transformation of biomass step by step into key chemicals for the further utilization have been massively conducted[3]. While during a series conversion process of raw biomass, Aldehydes are believed to be particularly troublesome for the aldol condensation and polymerization reactions, to avoid which, hydrogenation process is necessary. As an alternative to traditional high-pressure and -temperature processing, we are choosing electrochemistry that can operate in ambient condition for the conversion of benzaldehyde which is a typical biomass-derived chemical. Another reason of choosing benzaldehyde is that the hydrogenation products benzyl alcohol and hydrobenzoin and the oxidation product benzoic acid are important industry chemcals[4](Figure 2).

Based on related publications about benzaldehyde conversion by electrochemical method, using aqueous electrolyte, and catalysts such as Pd, Cu, Ni-based materials are the most efficient electrocatalysts for reduction of Benzaldehyde into Benzyl alcohol[5].

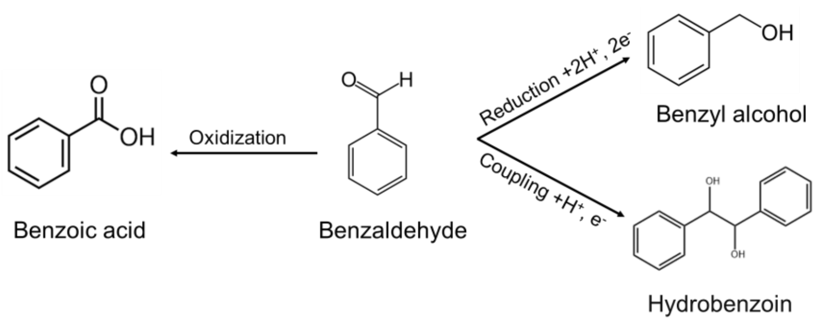

Figure 2. Electrochemical conversion of benzaldehyde

Meanwhile there are few reports of electrocatalysis of C-C coupling reaction of benzaldehyde using graphene and Cu, Pb as working electrodes. While some reports of photocatalysis of C-C coupling reaction with Cd, In, Ti, Zn element-based materials as photocatalysts[6].

As for the desired oxidation product benzoic acid, a new concept of low voltage oxidation is come up with[7]. Conventionally the voltage needs to put on anode is higher than 1V (vs. RHE), but the reaction also can occur much lower than that. The onset potential is only need higher than 0.05 V (vs. RHE).

Objectives

The general objective is to demonstrate that electrochemical conversion of benzaldehyde is the most suitable technology to take advance of biomass-derived chemical.

The specific objectives of the project are the following:

- Using scalable, clean and safe synthesis routes, to design and engineer high performance electrocatalysts for the conversion of benzaldehyde.
- Evaluate the electrocatalyst performance of derived product chemical toward electrocatalytic oxidation (ECO) and electrocatalytic hydrogenation (ECH), selectivity and stability under reaction conditions.
- Study the reaction mechanism using characterization tools and modelling.
- Develop a prototype electrochemical system where an oxidation and a reduction reaction are coupled.

- To effectively disseminate the project results through publications and international conferences, and by the PhD defense.

Work plan and time table

This research plan will last three years, from September 2021 to May 2024.

I will design, engineer and characterize high performance electrocatalysts based on highly efficient metals towards the conversion of Benzaldehyde into desired products with high efficiency, selectivity and stability. For that, we are considering to do electrocatalysis based on elements Pd, Ni, Cu supported on ofor benzyl alcohol and Cd, Zn, In, Pb whose performance towards C-C coupling of Benzaldehyde have been proved in photocatalysis. The oxidation process we will choose no-noble metals such as Cu, Ni-based materials to catalyze. To accomplish the goals of this highly interdisciplinary project, I will work in three research directions: 1) preparation of suitable electrocatalysts using scalable, clean and safe synthesis strategies; 2) optimization of individual electrocatalytic processes in three electrodes H-cell reactor; and 3) engineering prototype devices where the benzaldehyde reduction and oxidation reactions will be coupled.
Based on the complexity and ambition of the project and its objectives, the work plan is divided into 5 work packages (WPs):

WP1. Synthesis of electrocatalysts (M1-M24).

Description of work: I will design and produce oxidation and reduction electrocatalyst to test individual electrochemical reactions. To design the materials, we will consider Pd, Ni, Cu-based materials as electrocatalyst for electrocatalytic hydrogenation of benzaldehyde into benzyl alcohol or oxidization into benzoic acid and the Cd, In, Ti, Zn-based materials as active compounds for the reduction product Hydrobenzoin. Using H-cell reactor to evaluate the performance and using different electrolytes to obtain best condition. Structural and chemical characterization tools such as x-ray diffraction (XRD) will be used to obtain critical insights into the structure/property/function relationships and the nature of the active sites of the catalysts.
Output: Different sets of electrocatalysts as a key component to be used in the Electrochemical conversion of benzaldehyde.

WP2. Study of individual electrocatalytic reactions (M6-M30).

Description of work: Gain fundamental knowledge and experience in related electrocatalytic properties and devices. Provide feedback to optimize catalysts and to define the technical viability of electrochemical hydrogenation and oxidation of benzaldehyde.
Output: I will study individual electrochemical reactions associated to the valorization processes of benzaldehyde and using the electrocatalysts produced in WP1.

WP3. Design and engineering of electrochemical systems with coupled reactions and process parameter optimization (M6-M30).

Description of work: Development of prototype electrochemical systems operative for the simultaneous conversion of biomass platform chemical benzaldehyde via paired electrolysis. Now the flow reactor is more considered ideal type for the electrochemistry reaction in the lab for the reason that the flow reactor can keep high reaction rate and with a high Faradic efficiency. In my opinion, for the reaction like water splitting reaction it is good that we do not consider the product separation problem. But for the organic conversion reaction, especially occurred in aqueous electrolyte, it is inevitable we need to consider this. Therefor we are considering optimize this based on batch reactor (H-cell reactor) to reach high electron and ion transport rates. If it is possible, we hope it can have a potential industry application.

Output: Prototype system for paired electrocatalysis of benzaldehyde reduced into benzyl alcohol and oxidized benzaldehyde into benzoic acid.

WP4. Dissemination and exploitation of the project results (M12-M36).

Description of work: Based on data collected, write essays. Attend electrochemistry congress.

Output: At least one Q1 publication.

WP5. Write and defend my PhD thesis (M30-M36).

Description of work: To write an exceptional PhD thesis and defend it in front a jury composed of three worldwide experts in the field to obtain by PhD degree from the University of Barcelona.

Output: Write PhD dissertation and at the end of the project and defend it in front of an international jury of experts in the field of energy storage and particularly on electrocatalysis. Obtain the PhD thesis and PhD degree.

Time Schedule

WPs	Time table					
	6	12	18	24	30	36
WP1						
WP2						
WP3						
WP4						
WP5						

This project is planned to take place from September 2021 until the end of May 2024.

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Signatura:

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