Chemistry
Graduate Program

MASTER'S DEGREE IN CHEMISTRY
UNIVERSITÉ PSL

PSL UNIVERSITÉ PARIS

Internship proposal for Master in Chemistry Students at PSL

Title
Modelling the Response of Bi-Enzymatic Amperometric Sensors

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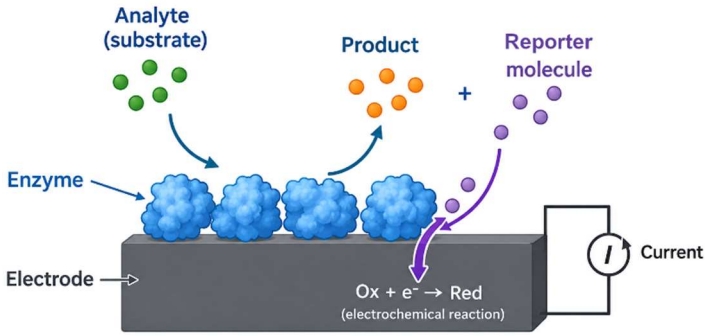
Topic description (context, objectives, techniques used, references)



Context: Electrochemical enzymatic micro-/nanosensors combine the advantages of electrochemical approaches (e.g., signals proportional to the analyte concentration, local measurements, etc.) with the specificity and efficiency of enzymes, which allow the conversion of the analyte of interest into a product and an electrochemically active reporter molecule (see figure). Enhanced mass transport at micro-/nanoelectrodes is generally a great advantage of these devices but can be counterproductive under certain conditions, leading to extremely fast escape of reporter molecules and thus decreased efficiency of analytical measurements [1, 2].
Modelling and simulations allow one to optimize the sensor's response, taking into account the constraints of a given platform (electrode dimensions, concentration range, enzyme kinetics, etc.). In many situations of interest, transforming the analyte of interest into an electrochemical reporter molecule requires more than one enzymatic step (see e.g., [3, 4]), making it even more difficult to achieve the balance between mass transport and enzyme kinetics, which is crucial for accurate analytical measurements.

Objectives/Description: The purpose of **this Master 2 research internship** is to model the responses of a bi-enzymatic amperometric sensor. At the beginning, a bi-enzymatic device, where both enzymes follow Michaelis–Menten kinetics, will be considered. If time permits,

more complicated mechanistic situations will also be modelled. Analysis of the obtained results should allow the identification of the parameters with the largest effect on the sensor's response, as well as their optimal ranges. Simulation results will be compared with experimental data available in the literature or from our collaborators. The modelling will be mainly performed in COMSOL Multiphysics software, as well as other numerical tools, depending on the project development.

Candidate profile: The ideal candidate should have a solid background in physical chemistry/electrochemistry (or a related field) and modelling. Knowledge of biochemistry and experience with numerical tools (e.g., Python, MATLAB, Mathematica) are a plus.

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Please send a CV and contact information for one or, preferably, two referees.

References:

[1] R. Dannaoui, X.-K. Yang, W.-H. Huang, I. Svir, C. Amatore, A. Oleinick. Importance of diffusional constraints for the quantitative evaluation of calibration curves of enzymatic micro- and nanoelectrochemical sensors. *Electrochim. Acta*, 473, 2024, 143425.

[2] R. Dannaoui, I. Svir, W.-H. Huang, C. Amatore, A. Oleinick. Modeling the detection of transient vesicular exocytotic release from single cells with cylindrical enzymatic nanoelectrodes. *Electrochim. Acta*, 508, 2024, 145214.

[3] P. Lopes, K. Kaewjua, S. Shipovskov, E.E. Ferapontova. Glucose and Glutamate Detection by Oxidase/Hemin Peroxidase Mimic Cascades Assembled on Macro- and Microelectrodes, *ChemElectroChem* 2024, 11, e202300682.

[4] Y. Wang, A. Pradhan, P. Gupta, J. Hanrieder, H. Zetterberg, A.-S. Cans. Analyzing Fusion Pore Dynamics and Counting the Number of Acetylcholine Molecules Released by Exocytosis, *J. Am. Chem. Soc.* 2024, 146, 25902−25906.