Sujet thèse / PhD subject 2024

Titre Thèse	**Quantum-electrochemistry detection of DNA-protein interactions for cancer screening**	
(Co)-Directeur	Fabrizio CLERI	E-mail : fabrizio.cleri@univ-lille.fr
(Co)-Directeur		E-mail :
(Co)-Encadrant (s)		E-mail :
Laboratoire	IEMN	Web : www.iemn.fr
Groupe(s)	Physique	Web :
Projet phare (principal)	Flagship Technologies for Health	
Demande thèse labelisée IEMN (Materials ou IoT Make Sense)	**Non**	
Financement demandé	Contrat Doctoral Etablissement	ULille ☐ Centrale Lille ☐ JUNIA ☐
	Région – Autre ☒ Préciser : GRAEL	Co financement (Préciser l'origine, demande en cours, acquis ou pas) :
Financement acquis ☒ **Financement partiellement acquis** ☐	Contrats de Recherche ☐ Préciser :	Autre ☐ Préciser :

Résumé du sujet :

One of the main causes of death for cancer patients is organ failure induced by metastasis development. The primary tumor spreads through the body by generating circulating tumor cells (CTCs), that is, cancer cells that detach from the tumor, and extracellular vesicles (exosomes, EV), which circulate within the bloodstream. Our research group at IEMN Lille is partner in an effort to develop an innova.ve, original family of **lab-on-chip (LOC) devices, aimed at detecting CTCs and EVs** with high efficiency. The core of the LOC device are **DNA aptamers carrying redox species**, which detect the presence of a cancer cell immobilized on the chip by quantum-tunnelling current fluctuations.

Experimental studies are complemented by **two key theoretical and computer modelling pillars**:

- **extensive all-atom molecular simulations, which must characterize the DNA aptamers; their bonding with the electrodes and redox molecules; their dynamical fluctuation trajectory in solution, under realistic conditions; the ligand-receptor interaction between DNA and the protein.**

- **quantum-mechanical electron transport simulations, which use as input the detailed information extracted from the molecular-scale dynamics of the redox species, to calculate the tunneling current as a function of the DNA-protein interaction, to be compared with the experiments.**

The two coupled theoretical/modelling endeavors constitute the subject of the PhD work, which will be realized in close collaboration with the experimental groups, notably the group in LIMMS/IIS Tokyo (Japan), where short visits may be planned during the course of the PhD. The PhD project has also an underlying, more fundamental motivation in furthering the molecular-scale understanding of the DNA-protein interactions, and quantitatively improving the modelling of electron quantum transport.

The successful PhD candidate must have a good background in **at least three** of the following areas: applied mathematics, computational modelling, fundamental physics, biophysics, statistical mechanics, molecular modelling, basic cell biology, bioinformatics.
Working knowledge of Linux/Unix, C/C++/Fortran, Python is a title of preference.