# PhD Offer IN DEVELOPMENT OF COMPACT MODELS FOR JOSEPHSON JUNCTIONS USING AB INITIO SIMULATIONS

Record number : OPR-1050

## Overview

**RESEARCH DIRECTION**

Dominique Drouin, Professeur - Department of Electrical and Computer Engineering

**INFORMATION**

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**ADMINISTRATIVE UNIT(S)**

Faculté de génie
Département de génie électrique et de génie informatique
Institut interdisciplinaire d'innovation technologique (3IT)
Institut quantique

**LEVEL(S)**

3e cycle

**LOCATION(S)**

3IT - Institut interdisciplinaire d'innovation technologique

## Project Description

Context: Superconducting circuits are one of the leading candidates for the implementation of practical quantum computers. In this context, Canada's first semi-industrial fabrication facility for superconducting circuits will soon be established at the Institut interdisciplinaire d'innovation technologique (3IT) at Université de Sherbrooke. This will involve the elaboration of a Process Design Kit (PDK) for academic and industrial users of the facility wishing to fabricate chips according to certain specifications. An important aspect in the success of this fabrication is the capability to predict device performance before fabrication using numerical simulations to avoid excessive trial and error. While classical components like capacitors, inductors, and resonators may be modeled efficiently with commercially available finite-element codes, properties of the Josephson junction are determined by quantum transport physics at the atomistic scale.

Research project: The aim of this thesis project is to develop compact models of Josephson junctions that include the impact of atomistic defects that are specific to the 3IT fabrication processes. Supported by the expertise of 3IT, IQ and Nanoacademic Technologies Inc. in the fields of fabrication, finite-element and atomistic simulation for superconducting circuits, the student will have to (i) perform atomistic simulations based on the Non-Equilibrium Green's Function Density Functional Theory (NEGF-DFT) technique, (ii) develop analytical models based on approximate approaches such as the WKB method to generate an accurate compact model for the devices, (iii) collaborate with experimentalists to compare experimental data for Josephson junction transport characteristics with analytical and numerical modeling data that take foundry-specific geometries and defects into account, and (iv) provide the numerical and theoretical skills necessary to integrate the Josephson junction's models into the 3IT PDK and combine it with Nanoacademic's QTCAD® software, leading to more predictive design and fabrication workflows.

Supervision & work environment: Under the supervision of Profs. Dominique Drouin and Dr. Aldilene Saraiva
, the work will be carried out mainly at the Interdisciplinary Institute for Technological Innovation (3IT) and at the Quantum Institute (IQ) of

UdeS, in close collaboration with the company Nanoacademic Technologies Inc. 3IT is a unique institute in Canada, specializing in the research and development of innovative technologies for energy, electronics, robotics and health. The IQ is a state-of-the-art institute whose mission is to invent the quantum technologies of tomorrow and transfer them to the industry. Nanoacademic Technologies Inc. is a small scientific software company based in Montréal. Founded in 2008 as a spin-out of research done by the group of Prof. Hong Guo at the McGill Physics Department, Nanoacademic develops and distributes atomistic and quantum modeling software for material science and nanodevice engineering applications. Nanoacademic is currently leveraging its finite-element and atomistic simulation backends to develop new design tools for superconducting circuits. The student will thus benefit from an exceptional research environment that combines students, professionals, professors, and industrialists working hand-in-hand to develop the future technologies.

Researched profile:
• Specialization in physics or computational material science
• Programming skills in Python (preferred) or another scientific programming language
• Strengths: knowledge in superconducting qubits and the physics of Josephson junctions
• Assets: experience in computational ab initio modeling techniques such as density functional theory or molecular dynamics
• Excellent adaptability, autonomy, teamwork, and problem-solving skills.
• Strong taste for theoretical modeling work with immediate applications to experimental physics and engineering.

Documents to provide: CV, all post-secondary transcripts and references.

## Discipline(s) by sector

### Sciences naturelles et génie

Génie électrique et génie électronique

## Funding offered

To be discussed

## Partner(s)

Nanoacademic Technologies inc.