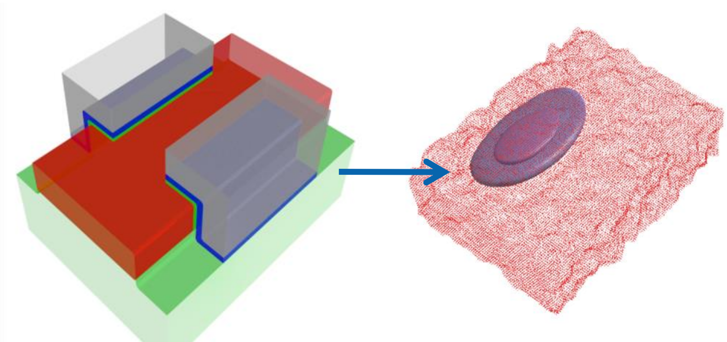
PhD position on the multi-scale modeling of materials and devices for quantum computing

A fully funded PhD position on multi-scale modeling for quantum computing is open at CEA Grenoble, France. The PhD is expected to start autumn 2021 and lasts three years.

“Quantum computers” are expected to solve problems beyond the reach of conventional computers. In a quantum computer, the information is not simply stored as a series of “0” or “1”, but as a coherent superposition of all possible states. The preparation, coherent manipulation and measurement of such quantum states is extremely challenging. One promising option for making quantum bits is to divert silicon metal-oxide-semiconductor (MOS) transistors to trap one or a few electrons, and use their spin to store and manipulate quantum information. The CEA Grenoble designs, fabricates, and characterizes such spin “qubits”, and develops a multi-physics code, TB_Sim, for the simulation of quantum materials and devices from the nano- to mesoscopic scales.



Models for two “face two face” quantum dots. On the left, finite elements model for the electrostatics (silicon in red, SiO_2 in green, HfO_2 in blue, and metal gates in gray). The metal gates control the potential in silicon; they can be used to trap, manipulate and “measure” electrons. On the right, atomistic model for the silicon wire, with the iso-probability surfaces of the first electron trapped under the left gate. Each red dot is a silicon atom at the surface of the wire.

However, a few limitations prevent modeling from being fully predictive on these devices. One of the main challenges is the description of surfaces, interfaces, and defects, which play an essential role in silicon. The aim of this thesis is, therefore, to introduce atomistic *ab initio* approaches such as density functional theory (DFT) in the chain of multi-scale simulations for quantum devices. The candidate will, in particular, address the connections between the atomistic and mesoscopic scales, and focus on the Si/SiO_2 interface and Si/Ge qubits and their defects as an application. Our ambition is to make numerical simulation predictive even on uncharted grounds, and to integrate it at all stages of the design, fabrication, and characterization of the qubits. For that purpose, numerical experiments will be performed to confront simulation with experimental observations, to provide the “missing pieces of the puzzle” that cannot be measured directly, and to give feedback to the design. This work will be carried out in close collaboration between CEA-Leti and CEA/IRIG. The candidate will also have the opportunity to collaborate with the partners of CEA in Europe.

The position is funded by a grant from CEA (net grant: ~1600 €/month).

The candidates must have a Master degree in quantum or solid-state physics and have strong computational skills. They shall send a CV, a letter of motivation and two contacts for references to:

Benoît Sklénard and/or Yann-Michel Niquet

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