

# What does modelling tell us about spin qubits?

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Silicon and Germanium spin qubits have made outstanding progress in the past few years [1-3]. In these devices, the elementary information is stored as a coherent superposition of the spin states of an electron or hole confined in a quantum dot embedded in a Si/SiO<sub>2</sub> or Si/Ge heterostructure. These spins can be manipulated electrically owing to spin-orbit coupling, and are entangled through exchange interactions, allowing for a variety of one- and two-qubit gates required for quantum computing and simulation.

The physics of spin qubits is particularly rich and complex. The spins undergo subtle interactions with the host materials and are very sensitive probes of the local electrostatics, strains and disorder. The design of the devices and the analysis of the experiments calls, therefore, for a comprehensive understanding of these interactions. In this context, modeling and simulation can provide invaluable insights into the physics and operation of spin qubits [2, 4-6].

In this tutorial, I will give an introduction to the modelling of spin qubits. I will discuss, in particular, two methods used to compute the electronic structure of quantum dots: the effective mass approximation and the tight-binding method. The latter can describe the qubits down to the atomic scale when needed (e.g., to capture the effects of defects, dopants, interface roughness, etc...). I will illustrate this tutorial with examples showing how modeling

reveals the exciting life of a spin in a quantum device. I will finally discuss the key challenges and opportunities for spin qubit technologies from the point of view of modelling.

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## References

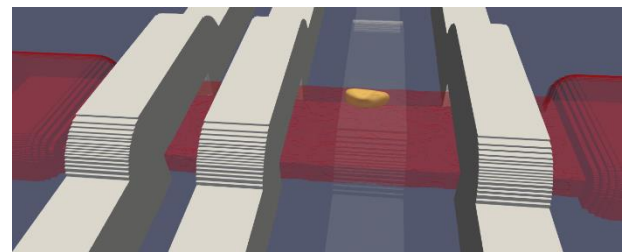
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## Figures

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**Figure 1:** Model for a silicon spin qubit [2]. The spin of a hole in a silicon channel (red) is controlled by metal gates (white). The yellow shape is an iso-density surface of the hole wave function.

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