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The never-ending demand for the progress in microelectronics has motivated the development of ultra-scaled transistors. The state-of-the-art transistors, lying at the heart of computers processors, have already reached the astounding dimensions of 14 nm. Nonetheless there is a continuing scientific effort to push this boundary even further, with the 5 nm fabrication process goal to be reached within next five years. Such dimensions correspond to less than 20 atoms stacked on top of each other. With that scale of miniaturization silicon transistors working properties are in fact determined by the presence of minuscule concentration of other atomic species: impurities (such a phosphorous) also known as dopants. Silicon technology is in fact now approaching a limit at which both the location and number of individual dopant atoms within an active region of transistor will determine its characteristics.

Controlling the precise position of dopants within a device and understanding how this affects device behavior have therefore become essential and may open a route towards novel future devices such as single-atom transistors. Devices based on the controlled positioning of single dopants in silicon are also primary candidates for solid-state quantum computing. Silicon in fact appears as an ideal environment for such applications. It can be enriched with high isotopic zero nuclear spin 28Si isotope, with almost negligible concentration of spin-carrying 29Si nuclei. The nuclear spin free 28Si host is known therefore as ‘semiconductor vacuum’ as it does not affect spin ‘coherence and relaxation time’ which are key features for efficient applications in quantum information.

These and similar results distinguish donor nuclear spins in silicon as the most coherent solid state quantum system, surpassing even atomic systems in vacuum. The vision of combining quantum spin control with the superb fabrication technology already utilized for classical computers has stimulated extensive effort in silicon-based quantum devices over the past decade. The new applications will use the unique quantum properties of single dopants. For example an electrically gated donor could be used to address and couple quantum bits. Controlled creation and manipulation of single dopants, as well as their utilization in novel devices has in fact opened a new field of solotronics (solitary dopant optoelectronics).

From a theoretical point of view a fundamentally new understanding and methodology is needed to model the operation of few-atom devices. In particular, when the dopant is taken out of the bulk crystal configuration and is put in a complex environment such as quantum well or quantum dot, or when fields are applied. In this project, we intend to formulate theoretical description and perform large-scale calculations of spectral properties of silicon nanodevices doped with single impurity atoms. Single dopant embedded in a host environment of millions of silicon atoms forms a complicated nanosystem where every atoms must be accounted for individually. In other words: every atom matters. Our approach will therefore utilize the atomistic tight-binding method that naturally incorporates effects of quantum confinement, external fields, and atomistic effects such as interfaces steps and composition disorder. We will parallelize our computational codes and run them on massively parallel computer clusters. We aim to apply our methodology to solve currently untraceable problems where impurity wave-function extends over ten millions of atomic sites. We expect to observe the effects of local environment, such as dielectric interfaces and quantum confinement of the dopants on their energies and lifetimes. Transport of charge through atom-based devices will depend on how the charge distributes in and flows through the individual atoms. We will run calculations for various nanodevices differing with the underlying dopant placement and number. Thanks to close collaboration with the National Institute of Standards and Technology (NIST) we will have the unique ability to correlate the measured and calculated data.

Our results will be highly relevant to the development of atomic-scale silicon transistors, and to the fabrication of single-dopant optoelectronic devices and spin-based quantum computation. Our theoretical analysis may help to determine the degree of confinement imposed by gates and address important issues of the control of the coupling between donors. It may also open a path to incorporation of quantum functionalities into state-of-the-art silicon devices through control of single donor wave function. We should reach level of understanding essential for engineering of addressable quantum bit operations in silicon donor devices. The proposed project may have not only important future industrial applications, but will allow for basic studies of confined many-body systems in solid-state environment.