# Behavior of Two Hole Qubits of Boron Atoms in Silicene

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**Abstract**
In this work, using the density functional theory in the framework of the spin non-collinear generalized gradient approximation, the behavior of the magnetic moments of B:Si hole center qubits was investigated. The spin dynamics, the charge density transfer, and the influence of these parameters on the total electronic energy of the system are calculated. The results obtained are promising for the design of a two-qubit quantum system as a logical gate for future quantum computers.

**Keywords 1**
Boron, qubit, silicene, electron density

## 1. Introduction

Due to the strong spin-orbit interactions of holes in a silicon system [1], hole systems are attracting active attention as possible objects for creating solid-state atomic systems for performing quantum computations [2]. Hole systems formed by impurity boron atoms in silicon are better amenable to electrical control (in comparison with the electron spin), and, on their basis, it is possible to create fast, well-tunable quantum qubits [3, 4]. The interaction of hole spins with each other in silicon occurs through short-range antiferromagnetic exchanges [5]. Further, it was shown [6] that the spin polarization of holes is also observed in the absence of an external magnetic field.

In this paper, using quantum mechanical modeling, we investigate the regularities of the behavior of the magnetic moments of the qubits of the B:Si hole centers. We study in detail their spin dynamics and the transformation of the charge density in their environment. The results obtained will help develop recommendations for experimenters and technologists engaging in the production of future quantum computers.

## 2. Methods and approaches

We used the Quantum opEn-Source Package for Research in Electronic Structure, Simulation, and Optimization (ESPRESSO) software code [7], by means of high-performance computing, for the modeling of silicene's atomic structure and the calculation of the total energy of B:Si systems. Perdew-Burke-Ernzerhof (PBE) fully relativistic ultrasoft pseudopotentials for silicon and boron atoms in the generalized-gradient approximation (GGA), with the spin-orbit interaction, were taken from the Quantum ESPRESSO package. The silicene unit cell, consisting of two silicon atoms, was placed in a cell measuring 3.845 × 3.845 × 12.490 Å in the shape of a straight prism. All atoms were given complete freedom. As a result of relaxation, an equilibrium model of impurity-free silicene was obtained. Then, using translational symmetry, a 6 × 6 × 1 supercell was constructed, consisting of 72

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silicon atoms. Then, the 72-atom model was placed in a 23.070 × 23.070 × 12.490 Å cell. A special k-point set of 2 × 2 × 1, with an energy cutoff of 476.20 eV, was used to calculate the silicene characteristics.

## 3. Results and discussion

To study the behavior of boron atom qubits in silicene, two silicon atoms were substituted by boron impurity atoms. For this, we chose two hexagonal rings located at the edges of the silicene monolayer so that the distances between the boron atoms were no less than 10 Å. For the purity of the computational experiment, the boron impurity atom was alternately placed in all six positions in the ring, and, after complete relaxation of the system, the total energy of the system was calculated for each position. All positions turned out to be energetically approximately equivalent to each other, so any of them could be chosen for further research. In this work, we present the calculation results for the B1 and B2 positions of the boron atom in silicene (Figure 1). Upon the incorporation of boron impurity atoms into silicene, an even greater distortion of its structure is observed. This is clearly demonstrated by the value of the angle Si – B – Si, which significantly increases in comparison with the system without impurities and was computed to be 119.55°. The length of the interatomic bond d(B-Si), on the contrary, decreased in comparison with the system without impurities and amounted to 1.949 Å. With increasing distance from the boron atom, the disturbances in the silicene structure begin to smooth out. Thus, if in the hexagonal ring closest to the boron atom, the angle Si – Si – Si averages to 118°, then in the next nearest ring, the angle is equal. The Si – Si – Si angle, on average, is already equal to 116.97°, which practically corresponds to the undoped structure.

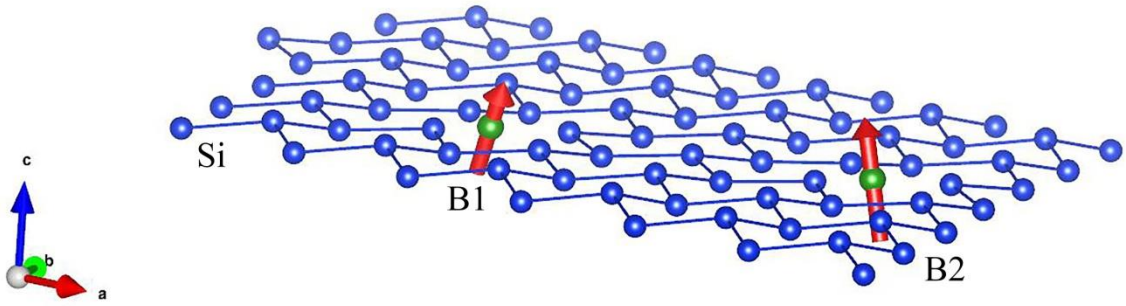


**Figure 1**: Model of modified silicene containing 70 silicon atoms and 2 boron atoms.

At the next stage of the work, we needed to investigate how the change in the angle, denoted θ, in the Bloch sphere between the z-axis and the magnetic moments of the boron atom affects the total energy, denoted $E_{total}$, of the system. For this, the magnetic moments on the B atoms were simultaneously deflected by equal angles of θ from the 0° base position (quantum state |0>) to 180° (quantum state |1>) with a step of 10°. It should also be noted that the initial angle θ and the angle obtained after the calculation differed from each other on average by a factor of two. So, for example, when setting the initial angle to θ = 10°, at the output, we arrived at θ = 5°. As a result of these calculations, curves were obtained showing the dependence, $E_{total}(\theta)$ (Figure 2).

Thus, it can be seen that the curves of the dependence of the total energy on the angle of rotation of the magnetic moments of B1 and B2 boron atoms in silicene behave in the same way, with the only remark being that the curve for B2 is wider. In the sections from 0° to 5° and from 175° to 180°, we observe a mirror-like abrupt growth of $E_{total}$, and then, in the sections from 5° to 55° and from 125° to 175°, we observe a further gradual increase in the total energy. Attempts to increase the value of the angle θ to 90° were unsuccessful. We believe that the fact is that in the region from 55° to 125°, the so-called spin blockade occurs, which is observed in double quantum dots [8]. This spin blockade prohibits the formation of a singlet state for magnetic moments on boron atoms. In addition, it should be noted that the graphical dependences of $E_{total}(\theta)$ indicate that the most favorable states for the

magnetic moments of the boron atom are quantum states |0> and |1>. The energy difference between these states is 0.28 μeV. These most favorable ground states for magnetic moments are triplet states.

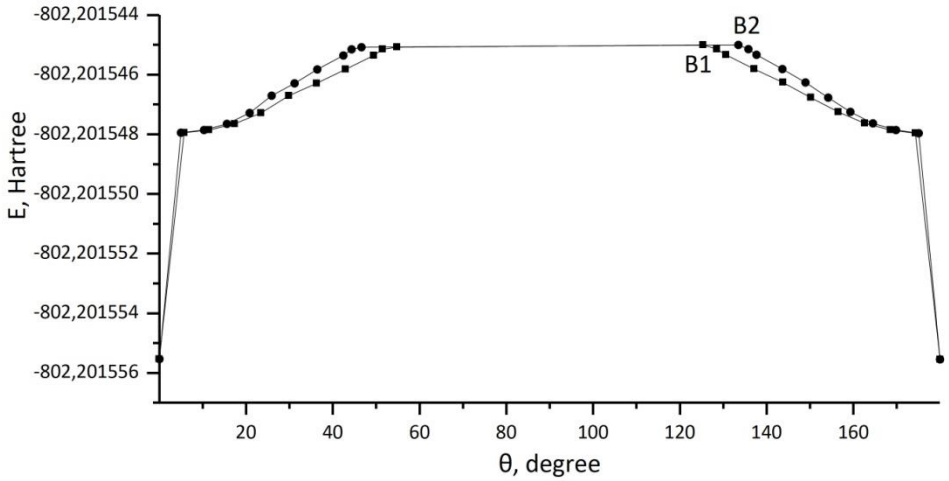


**Figure 2**: Change in the total energy, $E_{total}$, of the system, depending on the angle θ at different positions (B1 and B2) of the boron atom in the silicene structure.

Next, we investigated how the charge distribution density in the $Si_{70}B_2$ system was changed depending on the position of the magnetic moments of the boron atoms. For this, the differences in the charge density distribution at the main reference points of 0°, 5°, 55°, and 180° were calculated. These differences in charge density are shown in Figure 3, and they were obtained by finding the difference in charge density for each of the corresponding states. A detailed analysis of the spatial localization of the charge density showed a significant redistribution in the environment of the B1, B2, and neighboring silicon atoms due to the exchange interactions between the atoms.

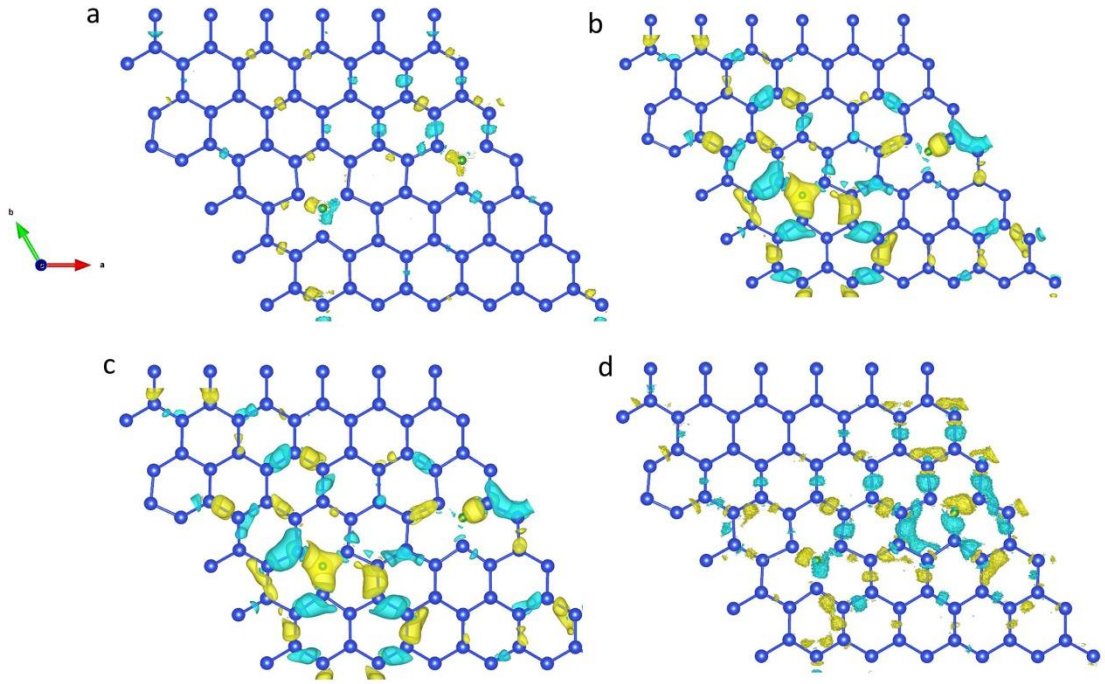


**Figure 3**: Charge density distribution for the following states in the $Si_{70}B_2$ system: (a) 5° – 0°, b) 55° – 5°, c) 55°– 0°, d) 180° – 0°).

Indeed, during the simultaneous rotation of the magnetic moments on the B atoms through an angle from 0° to 110°, the charge density increases on the B1 atom, on the B1 – Si bond, and on the

silicon atoms closest to it. However, on the second B2 atom, the charge density decreases. It turns out that the B1 atom and the nearest Si atom pull down the electron density from the B2 atom. With the rotation of the magnetic moments on each boron atom, in the range from 130° to 180° (where the angle between the magnetic moments of the B1 and B2 qubits varies from 260° to 360°), the opposite situation is observed. The charge decreases on the B1 atom and the B1 – Si bond with the nearest Si atom, and on the B2 qubit, the charge density increases. Thus, in this case, the B1 atom and the nearest Si atom give a charge to the B2 atom.

Figure 4 shows the change in the magnetization on each of the boron qubits depending on the angle. With the rotation of the magnetic moments on the boron atoms in the range from 0° to 110°, the magnetization decreases on the B atoms but increases on the B-Si bond and slightly increases on the Si atom. However, the opposite is observed when turning from 260° to 360°, where the magnetization increases on the B atoms and decreases on the Si atom and in the interatomic space on the B-Si bond. It can be seen that the magnetization on the left (B1) qubit, with an increase in the angle from 0° to 55°, first decreases from 0.019 to 0.013 $\mu_B$/cell, and then, with an increase in the angle from 125° to 180°, it increases from 0.013 to 0.019 $\mu_B$/cell. At the same time, on the second (B2) qubit, within the angle from 0° to 55°, the magnetization first falls from 0.023 to 0.018 $\mu_B$/cell, and then, with an increase in the angle from 125° to 180°, it increases from 0.018 to 0.023 $\mu_B$/cell. We see that the magnetization on the left qubit is about 20-30% less than on the right qubit. In our opinion, such a difference in the values of the magnetic moments is observed due to the anisotropy of the electron shells and the interference of the valleys in the Brullian zone [9]. Also, as previously mentioned, in the range from 55° to 125°, a spin blockade is observed.

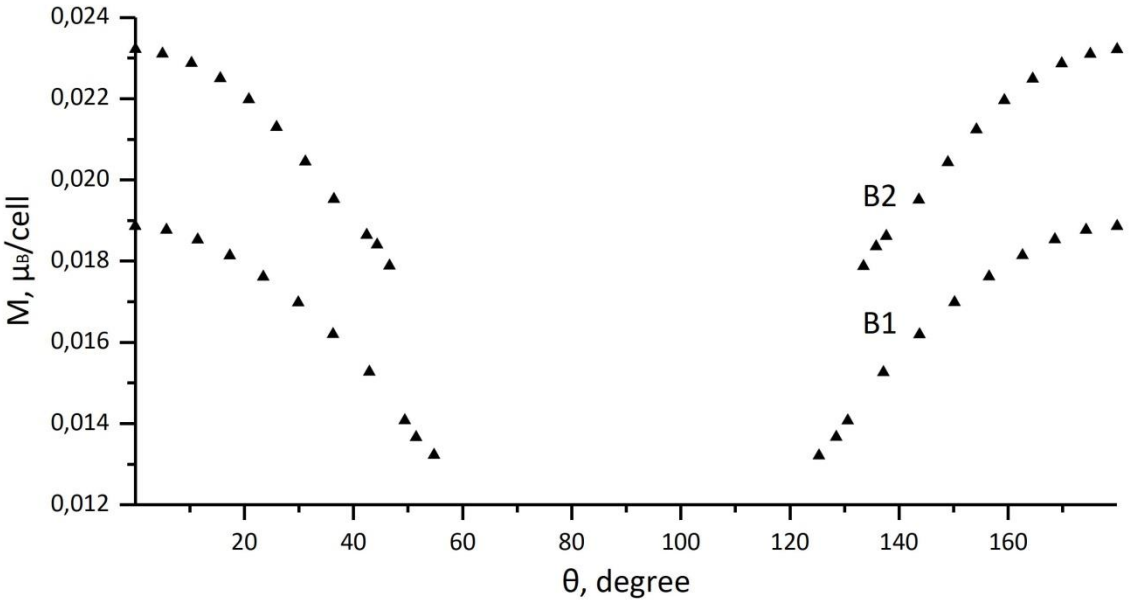


**Figure 4**: Changes in magnetization on each of the boron qubits, depending on the angle.

Thus, our results for the studied two-dimensional B:Si system are interesting and promising and can be used by technologists and experimenters to evaluate, design, and predict the physical properties of a two-qubit quantum system as a logical gateway for quantum computers.

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