

Quantum-mechanical prediction of the behavior of quantum trigger on a two-qubit cell of boron in silicene

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Abstract

The problem of creating energy-efficient quantum computers capable of performing quantum operations without errors is a significant scientific challenge in modern nanoelectronics. This type of computer can be developed using quantum transistors that contain hole qubits and are capable of performing operations on them. Hole qubits are a promising technology for quantum computers due to their strong spin-orbit interaction and the ease of control with an electric field. In this work, the influence of spin dynamics of boron impurities on the electron charge transport and electrostatic potential in a silicene structure is theoretically investigated using the noncollinear spin density method. To study spin dynamics, we calculated the dependence of the total energy change of the atomic system on the angle of rotation of the spin magnetic moments on boron atoms. It was shown that the two-dimensional system B:Si behaves as a quantum switch, allowing operations on the local distribution of charge density and electrostatic potential, thereby processing quantum information. The obtained results will be important for the technology of designing and manufacturing two-dimensional energy-efficient quantum computer.

Keywords

density functional theory, logic gates, quantum computing, silicon devices, two-dimensional hole gas

1. Introduction

Recently, solid-state nanoelectronics has been investigated the design of a quantum computer. These machines will accelerate the design processes of new materials with predetermined properties, enable fast drug development, and improve the systems of electronic and economic security, among other benefits. Quantum calculators can be built with logical gates (transistor) based on two qubits with a long coherence time, having fast control with a high precision of one- and two-qubit operations [1]. Such a logical gate can be obtained by introducing additional

boron atoms into the silicon structure [1–7]. Because of their strong spin-orbit interactions, hole qubits are more easily controlled by electric fields [1, 8] than by magnetic fields, so they operate faster than their electronic counterparts [9–13]. The physical implementation of quantum computing requires the control of each qubit in a quantum individual selective readout, as well as the combination of long-distance qubits, so that two-qubit gates can also be employed [14]. The Zeeman and Rashba spin splitting in two-dimensional (2D) hole systems is qualitatively different from their analogs for electronic systems, and spin-dependent phenomena in hole systems

can be obtained using the multipole expansion of the spin density matrix [15]. The hole spin interactions in silicon occur through short-range antiferromagnetic exchanges [16]. Thus, [17] found that the hole-spin polarization also takes place in the absence of an external magnetic field. This phenomenon was called the Dresselhaus interaction [18, 19].

In this novel work, we investigate the influence of the magnetic moment spin dynamics of B:Si hole-center qubits on the local charge density transfer and electrostatic potential changes in their environment using the spin-orbit non-collinear coupling method. The obtained results will explain the patterns of hole spin behavior, guide the design of a solid-state atomic device of the quantum calculator, and help to develop recommendations for experimenters and technologists for the future production of quantum computers.

2. Methods and approaches

All calculations of total energy and electronic properties were performed with the QUANTUM ESPRESSO software code [20]. Silicon and boron pseudopotentials in ultrasoft fully relativistic forms within the generalized-gradient Perdew–Burke–Ernzerhof approximation were used with the spin-orbit interaction and the spin polarization. The unit cell of silicene, consisting of two silicon atoms, was placed in a cell measuring $0.3845 \times 0.3845 \times 1.2490$ nm 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 including noncollinear magnetic states. Then, using translational symmetry, a $6 \times 6 \times 1$ supercell was constructed, consisting of 72 silicon atoms, and then placed in a $2.3070 \times 2.3070 \times 1.2490$ nm cell. A special k -point set of $2 \times 2 \times 1$, with an energy cutoff of 476.20 eV, was used to calculate the silicene characteristics. The atomic relaxation was carried out to interatomic forces of values up to 0.26 eV/nm of the resulting model had a hexagonal monolayer from Si atoms with a corrugated structure. The average layer curvature radius was 0.044 nm. The average length of the interatomic bond

Si–Si was 0.22626 nm, and the angle was 116.36° . These results aligned with the theoretical data of other authors [21]. The analysis of the atomic structure and charge distribution of the calculated structures was carried out using the Vesta software package [22].

3. Results and discussion

To assess the electronic structure of hole qubits created by boron atoms in silicene, two silicon atoms were replaced by boron atoms. Boron atoms were at least 0.10 nm from each other. Implanted boron atoms formed two holes in the silicene structure, the localization of which, surrounded by impurity boron atoms, is shown in Fig. 1. To study the spin dynamics, we calculated the dependence of the total energy change of the atomic system as a function of the rotation angle of the atomic magnetic moments on the boron atoms. Indeed, according to Bloch's notation, the orientation of the atom magnetic moment in space can be characterized by the magnitude of the magnetic moment vector and the angle θ of this moment with respect to the z -axis and the angle φ between its projection onto the xy -plane and the x -axis [23]. Thus, we calculated this change in the total energy from the angle θ , and the angle φ was assumed to be zero. For this, the magnetic moments on the B atoms were simultaneously deflected by equal angles θ from the $|0\rangle$ (0°) to $|1\rangle$ (180°) ground states with a 10° step. Figure 2 shows the change in the total electronic energy of an atomic system depending on the magnetic moment angle at each of the B atoms.

The curves of the magnetic moments of B1 and B2 boron atoms in silicene behave similarly. In the intervals from 0° to 5° and 175° to 180° , we observe a mirror-like abrupt growth of E_{total} , and then, in the sections from 5° to 55° and 125° to 175° , a gradual increase in the total energy occurs. Further attempts to increase the angle θ to 90° were unsuccessful likely because, in the region from 55° to 125° , a “spin blockade” occurs, which is observed in double quantum dots [24]. This spin blockade prevents the formation of a singlet state for magnetic moments on boron atoms. In addition, according to the graph of the

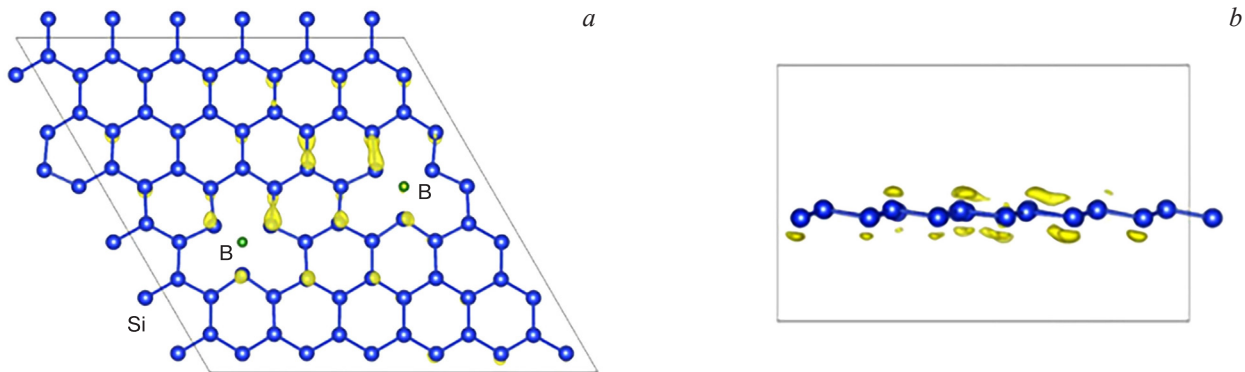


Figure 1. Localization of two hole qubits in the structure of boron-doped silicene: (a) along the $\langle 001 \rangle$ direction and (b) along the $\langle 100 \rangle$ direction

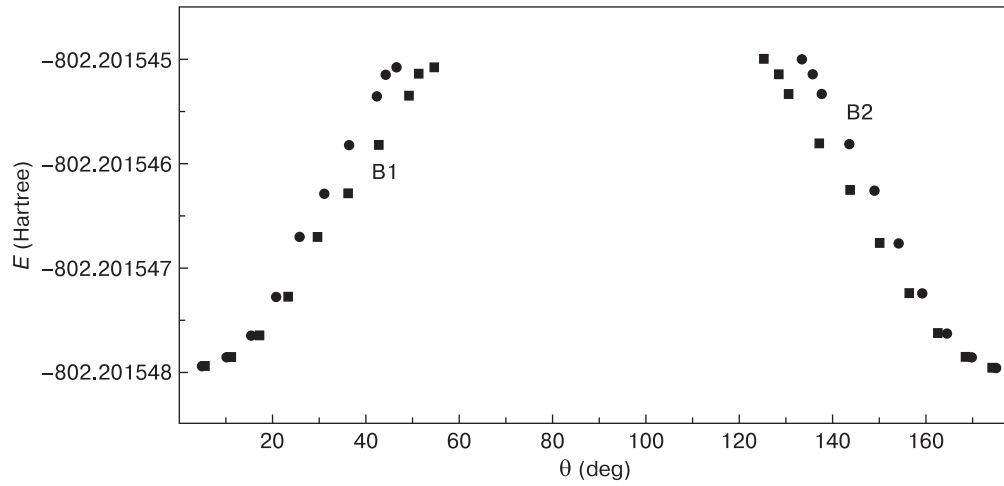


Figure 2. Total energy E_{total} of the system depending on the angle θ for magnetic moments of the boron atom in the silicene structure

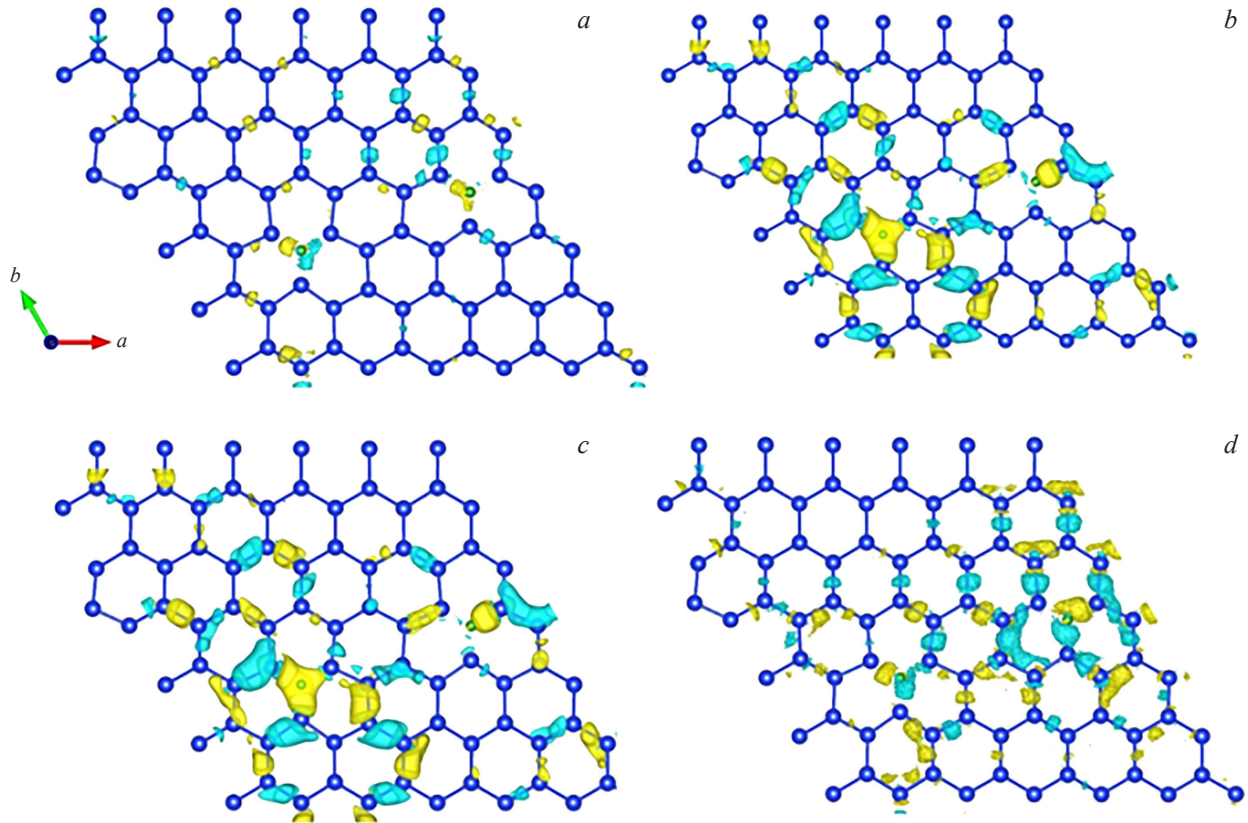


Figure 3. Difference density of charge distribution for system states Si_{70}B_2 : (a) $5^\circ-0^\circ$, (b) $55^\circ-5^\circ$, (c) $55^\circ-0^\circ$, and (d) $180^\circ-0^\circ$

dependence $E_{\text{total}}(\theta)$, the most favorable states for the magnetic moments of the boron atom are the quantum states $|0\rangle$ and $|1\rangle$. The energy difference between these states is $0.28 \mu\text{eV}$. These most favorable ground states for magnetic moments are triplet states. The magnitudes of the magnetic moments for these two qubits differ, owing to the anisotropy of the electron shells and the interference of the valleys in the Brillouin zone [25] and spin blockade.

Next, the change in the distribution of the charge density in the Si_{70}B_2 system was investigated based on the

position of the magnetic moments on the boron atoms. For this purpose, the differences in the distribution of the charge densities at the main reference points of 0° , 5° , 55° , and 180° were calculated, as shown in Fig. 3, by finding the difference in charge density for the corresponding states. A visual analysis of the spatial localization of the charge density showed its significant redistribution in the environment of the B1, and B2 atoms and the nearest silicon atoms, owing to the exchange interaction between the atoms. Indeed, when the magnetic moments on the B atoms are rotated simultaneously from 0 to 110° , the charge

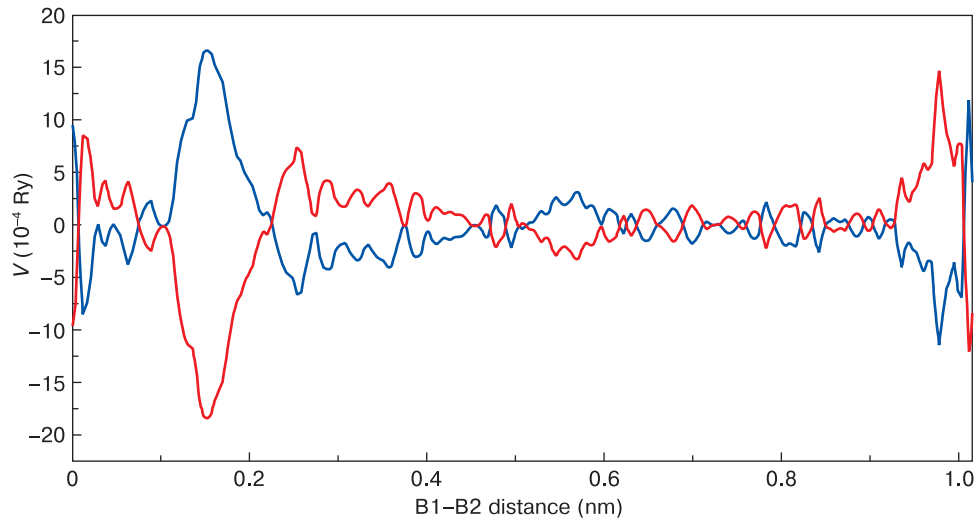


Figure 4. Electrostatic potential change between quantum B1 and B2 qubits' rotation of magnetic moments from 0° to 110° (red) and 260 to 360° (blue)

densities on the B1 atom, B1–Si bond, and closest silicon atoms increase.

However, on the second B2 atom, the charge density decreases. The B1 atom and the nearest Si atom seemingly pull down the electron density from the B2 atom. With the rotation of the magnetic moments on each boron atom from 130° to 180° (the angle between the magnetic moments of qubits B1 and B2 varies from 260° to 360°), the opposite situation is observed. The charges decrease on the B1 atom and the B1–Si bond with the nearest Si atom. 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.

Next, we analyzed the change processes in the electrostatic potential in this system with a change in the magnetic moment directions on the atoms (Fig. 4). We found that when the magnetic moments on the boron atoms rotate from 0° to 110°, the magnitudes of the electrostatic potential decrease on the B atoms and on the nearest Si atoms. Additionally, the potential grows on the B–Si bonds that are in the immediate vicinity of the B atoms. Thus, the hole localization sites shift closer to the boron atoms. In the case when the magnetic moments on the B

atoms are rotated from 260° to 360°, the opposite situation is observed. The potential grows on the boron and the nearest silicon atoms, and the holes move closer to the Si atoms.

4. Conclusion

In conclusion, in this work, theoretical studies of magnetic moment spin dynamics of B:Si hole-center qubits were carried out. We calculated the influence of the spin dynamics on the electron-transfer process and determined the regularities of changes in the electrostatic potential in the environment of hole centers. Thus, the obtained novel physical characteristics show that the considered system with two boron qubits located in the silicene lattice behaves like a quantum switch that allows operations on the local distribution of the charge density and electrostatic potential. Therefore, the transformation of quantum information can occur. Technologists and experimenters can use this 2D system and noteworthy results to evaluate, design, and predict the physical properties of a two-qubit quantum system as a logical gate for quantum computers.

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