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Modelling of Quantum Qubit Behaviour for Future Quantum Computers

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This work deals with quantum qubit modelling based on a silicon material with embedded phosphorus atoms because a future quantum computer can be built on the basis of this qubit. The building of atomic models of bulk crystalline silicon and silicene, as well as calculation of their total energies, were performed using the Quantum ESPRESSO software package, using highperformance computing (HPC). For silicon and phosphorus atoms the generalized gradient approximation (GGA) was used in terms of the spin-orbit non-collinear interaction by means of the Quantum ESPRESSO package. The equilibrium orientations of the phosphorus qubit spins and localization of the wave functions in the 2D and bulk crystalline silicon phases were theoretically investigated by means of quantum-mechanical calculations. The existence of an exchange interaction between qubits has been confirmed, which leads to a change in the wave function's localization and spin orientation, and in the case of silicene, this interaction was stronger.

Keywords: quantum qubit, quantum computer, quantum-mechanical calculations, spin.

Introduction

The problem of practical implementation of quantum computers is an important scientific and technological task at present time. The quantum computer will be able to instantly solve such important challenges as designing modern materials with specified properties, creation of new types of drugs, new types of cryptographic encryption, and also to significantly improve the work of machine learning and artificial intelligence systems. Over the past 10 years, various research groups have actively attempted to study and construct a quantum point qubit based on the spin in silicon [8]. Some groups have used the technological scheme proposed by Kane in 1998 [6]. According to this scheme, qubits are formed from long-lived nuclear spins of single phosphorus impurities in the Si crystal and are controlled by external surface radio-frequency, magnetic and electric fields. The spin states of an electron bound to one phosphorus donor in silicon show a long time of consistency and relaxation. Then, for the first time, Marello with co-workers [7] reported the possibility of the spin orientation readout in silicon. This allowed giving a further powerful impetus for an active study of spin orientations in silicon [9]. After that, a numerical model was developed for investigating electron-spin transfer through donors in silicon [5]. The authors showed that there are surprising effects that arise due to the quantization of phosphorus nuclei donors. They showed how it is possible to display the electron-exchange interaction using simple transport measurements. Thus, in Ref. [10], a behaviour of one- and two-qubit operations in a quantum point system using the exchange interaction was demonstrated. According to the latest data, researchers are trying to achieve a controlled overlap of the wave function for high-accuracy readout of spins on each qubit. Thereby, in Ref. [2] anticorrelated spin states between two donor spin-qubits in silicon located at a distance of 16 $\pm$ 1 nm were obtained. The authors have shown that the exchange interaction can be turned "on" and "off" by means of an electric field controlling the two phosphorus atoms.

This work deals with quantum qubit modelling based on a silicon material with embedded phosphorus atoms because a future quantum computer can be built on the basis of this qubit. To form the physical foundations of the quantum computer behaviour, it is necessary to study

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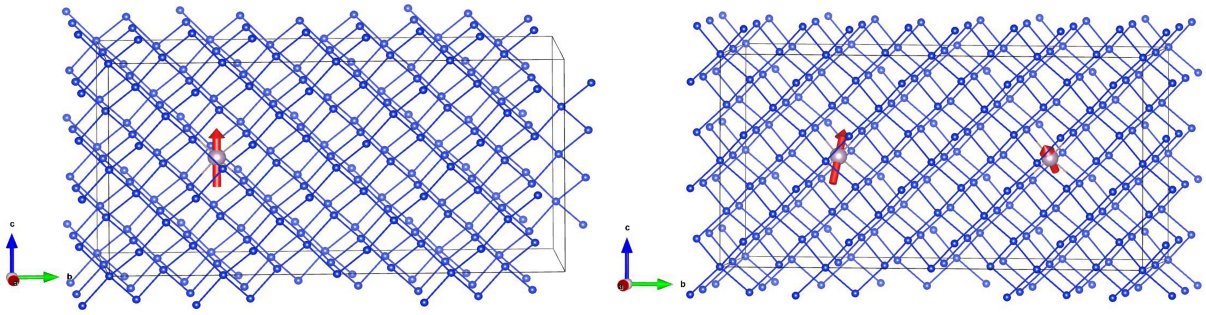
a model system based on a silicon material with embedded phosphorus atoms. Moreover, it is necessary to accurately describe the phosphorus impurity behaviour in a silicon matrix. The results will provide accurate data on the quantization and transmission of quantum information by means of spins.

1. Methods and Approaches

The building of atomic models of bulk silicon and silicene, as well as calculation of their total energies, were performed using the Quantum ESPRESSO software package [4], using high-performance computing (HPC). PBE (Perdew–Burke–Ernzerhof) pseudopotentials for silicon and phosphorus atoms in the generalized gradient approximation (GGA) in terms of the spin–orbit non-collinear interaction are taken from the Quantum ESPRESSO package. Calculation of a unit cell of bulk silicon was performed taking into account the $8 \times 8 \times 8$ k-points. For silicene, a special set of $9 \times 9 \times 1$ k-points was used with the 476.2 eV cut off energy of plane waves. The equilibrium silicene model was obtained by free relaxation of all atoms in the structure. For this purpose, the 32-atom model was placed in a cell with a size of $15.467 \times 15.467 \times 12.490$ Å^3. Atomic relaxation was carried out to the interatomic forces value of about 0.026 eV/Å.

2. Results and Discussion

During an implantation of one phosphorus atom (we denote it as 1P) into the bulk silicon lattice, the orientation "↑" is observed for the spin of the P atom's excess electron (see Fig. 1a). Adding a second impurity phosphorus atom (designated as 2P), at a distance of about 11 Å from the first one, leads to a change in the spin orientation of the 1P qubit (see Fig. 1b). It rotates to the $(\theta, \varphi) = (24°, -160°)$ angles (according to the notations in the Bloch sphere [1]). The second phosphorus atom has an orientation equal to $(\theta, \varphi) = (42°, -22°)$. Figure 2a shows the localization probability $|\psi|^2$ of the excess two electrons for the simultaneous presence case of 1P and 2P qubits in the silicon lattice.

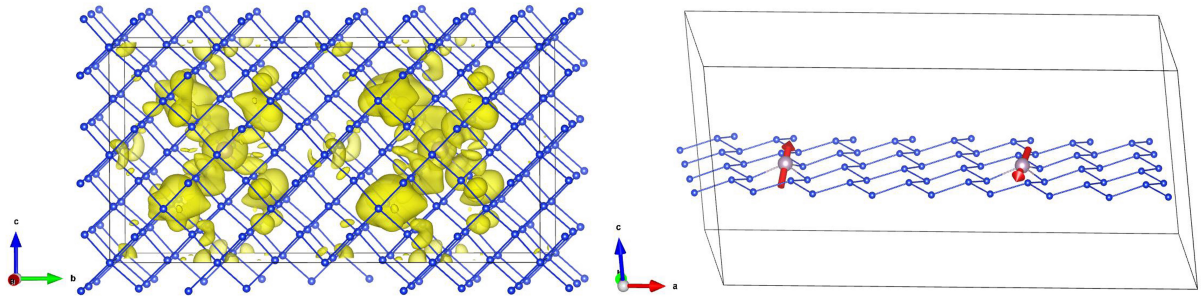


(a) for the case 1P

(b) for the case of the 1P (left) and 2P (right) atoms

Figure 1. The excess electron-spin orientation of the P atom

Then, we have calculated the equilibrium structure of pure silicene. The defectless silicene has the following geometric parameters (for the diatomic basis): $a = b = 3.867$ Å, the Si–Si interatomic distance is 2.270 Å, and the corrugation parameter is $d = 0.410$ Å. These parameters are in good agreement with the literature data: $a = b = 3.884$ Å; d(Si–Si) = 2.280 Å [3]. The phosphorus atom implantation into the silicene structure (at the 1/32 concentration) leads to its



(a) the silicon lattice (b) the silicene

Figure 2. The $|\psi|^2$ density in the silicon lattice and the spin orientations in silicene

strong distortion. The bond lengths slightly increase compared to pure silicene and, on average are Si–Si ≈ 2.275 Å, Si–P ≈ 2.285 Å. The θ_{SiPSi} internal angle for the phosphorus-doped silicene significantly decreased to approximately 109.6°. In pure silicene, the θ_{SiSiSi} angle was 116.8° on the average. During the one phosphorus atom implantation (1P) into the silicene lattice for the P electron spin, the "↑" orientation is also observed. The addition of a second phosphorus atom (2P) at a distance of about 15.467 Å from the first one leads to the spin orientation change of the 1P qubit as in bulk material. In this case, the 1P qubit spin turns to $(\theta, \varphi) = (43°, 95°)$ angles (see Fig. 2b). For the second phosphorus atom the orientation is $(\theta, \varphi) = (120°, -85°)$.

Thus, there is an exchange interaction between the two 1P and 2P qubits, leading to a localization change of the wave functions, spin orientation, and local charge density distribution. Besides, in case of the 2D silicon phase (silicene), this interaction is stronger because there is a greater deviation of the qubit spins' directions from the equilibrium orientations. We believe that the obtained results have a prospective significance for their use in the qubits design technology for future quantum computers.

Conclusion

We have used first-principles calculations to investigate the equilibrium orientation of the phosphorus qubit spins in 2D and bulk silicon phases. The localization of the wave functions and spin orientations were studied in detail. The results indicate that there is an exchange interaction between the two 1P and 2P qubits, leading to a localization change of the wave functions, spin orientation and local charge density distribution. Besides, in case of the 2D silicon phase (silicene), this interaction is stronger.

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