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Electronic Structure of Phosphorous Doped Bulk Silicon and Its Use for Spin Qubits for Quantum Computation

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ABSTRACT We have studied the electronic structure of silicon dopants which is necessary for implementation of spin based qubits in silicon. Description of dopant in silicon is therefore useful both as a benchmark and for determining the details of the electronic structure of an isolated dopant which can subsequently be used to calculate more accurate spin dependent scattering cross sections. These calculation have been able to perform large scale calculations using the computational resources. We have performed two electron Hartree-Fock calculations within effective mass theory. These efforts include calculating the effects of applied electric and magnetic fields and the coupling of two donors via exchange interaction. Tight binding calculations have also been performed including a calculation of the quadratic stark coefficient of the hyper interaction. We have found an unprecedented level of structure in the doping potentials and densities and wave functions. Due to oscillatory nature of doping potentials, the exchange coupling between qubits obtained by extrapolating our results to smaller distances was found to be less than estimates based on the Heitler-London approximation. The obtained results were found in good agreement with previously obtained results.

KEYWORDS Electronic structure, Dopant, isolated scattering, effective mass, quadratic stark coefficient, interaction, doping potential, qubits.

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INTRODUCTION

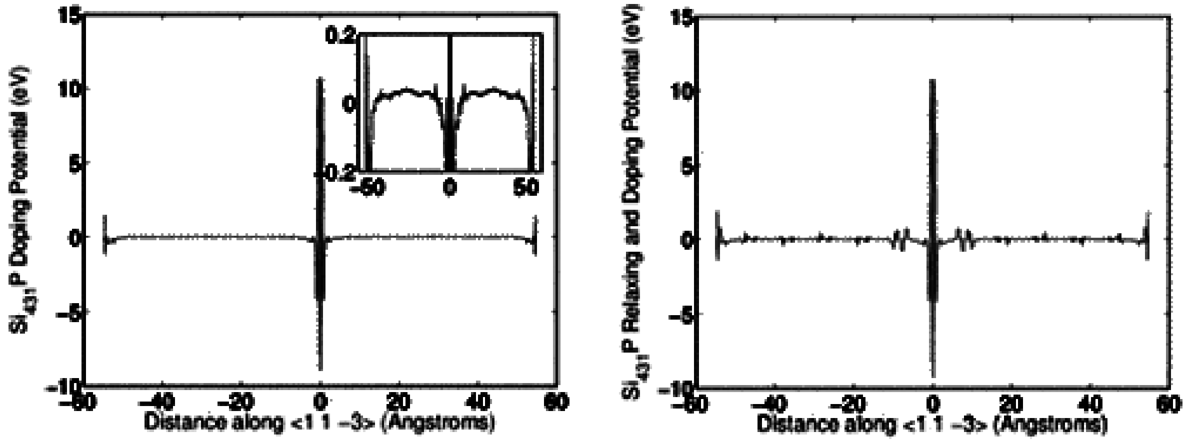
Kohn and Luttinger [1] studied that the theory of group-v dopants such as phosphorus in silicon is useful for describing the quantum nature of the electrons in these systems as well as for developing schemes to circumvent one of the most challenging aspects of solid-state quantum computers, namely environmental decoherence [2-5]. In order to provide a bench mark for such theories and also to use as a starting point for building efficient and accurate tight binding methods, an ab initio description of dopants in silicon is desired. The size of the systems required to describe doped silicon at or near the single dopant limit is large, making such a description computationally expansive. In this work, we have presented large scale density functional theory calculations for phosphorous doped silicon suprecells with up to 432 atoms. We have made comparisons to other theoretical works [6-9] to determine what can and cannot be captured by approximate or single-electron theories for the doped silicon systems. Previous efforts to describe the electronic structure of silicon dopants included effective mass approaches beginning with the work of Kohn and Luttinger and continuing with many others [10-15] including Fang etal, who performed two electron Hartree Fock calculations within effective mass theory [16]. Tight binding calculations have also been performed [17-19] including a calculation of the quadratic stark coefficient of the hyperfine interaction which has reproduced experimentally measured values more accurately than effective mass theory [20]. Density functional theory studies [21] evaluated the use of mixed Pseudopotentials which treated the dopant and silicon atoms in the layer using the same core potential and compared them to all atom calculations. These density functional theory calculations and a number of additional calculations [22] showed a large amount of disagreement for calculated properties such as the valley splitting.

METHOD

Face-centered cubic lattices of doped silicon were considered for variable dopant ratios by substituted one phosphorous atom in unit cells with 53, 127, 249 and 431 silicon atoms. We have used Perdew-Burke-Ernze-rhof density functional with an ultrasoft Pseudopotential for phosphorous and a norm-conserving Pseudopotential was calculated using FHI98PP for silicon. A plane wave energy cutoff of 65 Ry was chosen based on convergence of the total energy and pressure in the smallest supercell- K-space sampling was performed using a Monkhorst pack grid of $8\times8\times8$ of 54 atoms, $6\times6\times6$ of 128 atoms $4\times4\times4$ of 250atoms and $2\times2\times2$ of 432 atoms grid points. For the energy and properties of bulk silicon, a two atom silicon cell was used with a grid of $20\times20\times20$ k-points. In this cell one silicon is placed at the origin and another is placed at the point $\left(\frac{a}{4},\frac{a}{4},\frac{a}{4}\right)$ where a is the lattice constant. The basis vector of the fcc cell are $\left(\frac{a}{2},\frac{a}{2},o\right)$, $\left(\frac{a}{2},o,\frac{a}{2}\right)$ and $\left(o,\frac{a}{2},\frac{a}{2}\right)$, the two silicon atoms are repeated at every integer multiple of the basis vectors. The lattice constant of the doped supercells was determined as multiples of the 5.46Å lattice constant for bulk silicon computed with the Pseudopotential used in this stuydy. The phosphorous dopants repeat along the directions of the basis vectors. The Gram Schmidt procedure was used to find the orthogonal direction. $([-1\ 2\ 0])$. In the calculations with $N < 432$ atoms, all of the atoms were allowed to move during the simulation.

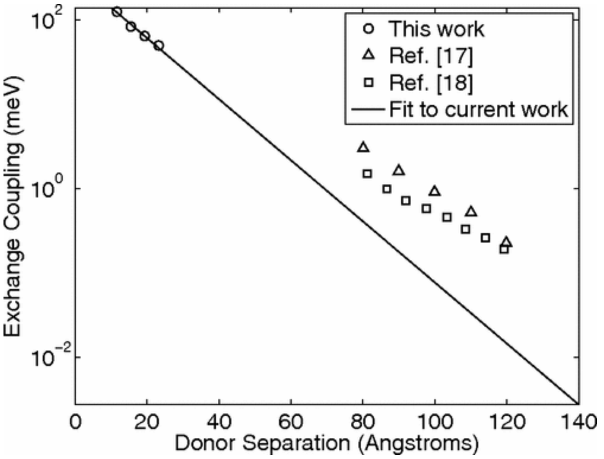
RESULTS AND DISCUSSION

Graph (1) shows the plot of the doping potential as a function of distance from (001) layer of dopants. In graph (1) (a) a full two dimensional cut through the potential is given in the plane perpendicular to the (001) plane, and the in graph (1)(b) and (1)(c) the potential is shown in a slice of this plane which connects two dopants. In graph (2) the mixed Pseudopotential doping potentials are much smoother then in graph (1) (b), especially in the region around the dopant. In graph (1) (b) there is a significant amount of structure in the potential near the dopant itself. Minor effects of the silicon atoms in the next layer of the crystal are also evident in graph (1) (c) when the effects of geometric relaxation are included. These results are for doping densities near the single dopant limit, a study of the effect of δ -layer of dopants would require very large cells which would likely have thousands of atoms. Additionally, the dopant potentials are plane averaged while we have plotted straight point potentials. Averaging does not eliminate the structure in our potentials but instead reduces the peak potential relative to the somewhat noisy structure of the atomic lattice. Oscillations are due to interactions with electrons in the shells below the valence shell. If these calculations were performed without using Pseudopotentials, which reduce oscillations from core electrons and replace them with a smooth potential the potential would most likely oscillate to an even greater degree. These oscillations, as well as possible in optimized geometries due to the silicon lattice distortions represent qualitative differences between density functional theory and effective mass theory. Mixed Pseudopotential in order to estimate the potential as a function of the distance from a layer of dopants. The obtained results were compared with previously obtained results of theoretical and experimental research works and found in good agreement.



(b) (c)

Graph 1: The doping potentials $\left(V_{si_{431}P} - V_{si}\right)$ as function of distance from the doping layer.



Graph 2: Magnitude of the zero-field exchange coupling calculated by density functional theory in this work (Circles), and in the Heitler-London approximation with effective mass theory wave functions.

CONCLUSION

We have studied electronic structure of phosphorous doped bulk silicon and its use in spin qubits for quantum computation. Several properties relating to their use as spin qubits for quantum computation were found. We have found that the electron density around the dopant leaded to non spherical features in the doping potentials, such a trigonal lobes in the (001) plane at energy scales of +12 eV near the nucleolus and of -700 meV extending away from the dopants. These features are generally neglected in effective mass theory and affected the coupling between the donor electron and the phosphorous nucleus. Our density functional calculations reveled in the densities and potential of the dopants which are not evident in calculations that do not include explicit treatment of the phosphorous donor atom and relaxation of the crystal lattice. The doping potentials provide input for scattering calculations, including calculations in which the current carrying electrons are confirmed to a two dimensional plane to model electrical readout schemes for silicon quantum computation. The obtained results were found in good agreement with previously obtained results.

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