Theoretical investigations of spin-orbit coupling effects on hydrogen-like donor states in bulk silicon and silicon nanocrystals

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Electronic properties of hydrogen-like donors in silicon are intensively studied since the middle of the previous century [1], including influence of the spin-orbit coupling on the donor states [2]. It is known, that spin-orbit interaction splits the $1s(T_2)$ donor state in bulk silicon (the so-called "spin-valley" splitting) [3]. This splitting was measured experimentally for group V antimony and bismuth donors [4] and singly ionized deep group VI donors, such as S^+, Se^+ and Te^+ [5]. Of course, some theoretical calculations were performed (for example, in [5]) to explain experimental results, but they were based just on the values of corresponding atomic spin-orbit parameters. However, strong influence on the donor states is induced by silicon matrix [6].

In this work combining envelope-function approximation and **k·p**-method with first-principles impurity potentials we theoretically study influence of the spin-orbit coupling on the structure of the ground state of some shallow and deep hydrogen-like donors in silicon. We have calculated spin-valley splitting for isocoric P^0 and S^+ donors and nonisocoric As^0 donor. The computed values are approximately 0.02, 0.3 and 0.12 meV for P^0, S^+ and As^0, respectively. As a test of our calculations' applicability we use experimental value of the spin-valley splitting for $Si:S^+$, which is approximately 0.36 meV [7]. Unfortunately, experimental observation of the spin-valley splitting for phosphorus and arsenic donors in bulk silicon using optical techniques is difficult because of their small values.

However, valley-orbit splitting of the donor electron 1*s* ground state sufficiently increases in silicon nanocrystals with typical sizes from 2 to 6 nm due to the quantum confinement effect [8]. We have calculated the spin-valley splitting of the $1s(T_2)$ state in doped silicon nanocrystals for phosphorus, singly ionized sulfur and arsenic donors, taking into account also interband spin-orbit coupling [9], and found sufficient increase of their values up to an order of a magnitude. So, in silicon nanocrystals investigated quantity in case of phosphorus and arsenic donors may become available for experimental observation.

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