

DFT Simulation of electronic and spin properties of GeV⁻ color center in volume and near-surface of nanodiamond for Temperature Sensor applications

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The „germanium-vacancy“ (GeV) center in diamond can be used as Temperature Sensors. The idea of GeV-based thermometry is based on optical measurements of the spectral shift of the zero-phonon line and its spectral width as a function of temperature changes. At the same time optical characteristics of GeV center which is located near-surface could be modified by formation of defect states in the band gap based on surface impurities and dangling bonds. The electronic structure of the GeV center determines its optical properties. The goal of this study was to investigate comparatively the geometric characteristics and electronic structure of the GeV center in the volume and near-surface (100) of nanodiamond in cluster approximation. It was shown for the first time that formation of isolated dangling bond on the (100) diamond surface leads to formation of unoccupied state in the band gap in vicinity of 1 eV, which is located on the distance of 1.9 eV of conduction band edge. This state in the band gap may influence optical properties of GeV in diamond.

Keywords: germanium-vacancy (GeV) color center, nanodiamond, electronic structure, surface states, dangling bonds, density functional theory.

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