Effect of Doping and Annealing on Structural and Optical Properties of Zinc Selenide Nanoparticles

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This study aims to explore the effect of doping and annealing on structural and optical properties of zinc selenide nanoparticles. The pristine zinc selenide nanoparticles (PZSNP), Nickel (Ni)-doped zinc selenide nanoparticles (NDZSNP), and annealed zinc selenide nanoparticles (AZSNP) have been prepared through solvothermal method. The surface morphology, structural and optical properties of the synthesized samples was analyzed by scanning electron microscopy (SEM), X-ray diffraction (XRD), and UV-visible spectrometer respectively. The SEM images demonstrated that the particle size increases in case of NDZSNP and AZSNP in comparison to PZSNP. The observed three XRD diffraction peaks corresponding to (111), (220), and (311) planes indicate the single cubic phase formation of all the samples. At higher DC up to 12% and annealed at higher temperatures up to 573K, the peak intensity increases significantly thereafter it decreases.In optical analysis, the absorbance of the prepared NDZSNP and AZSNP decreases whereas the refractive index increase as compared with PZSNP. With the increment of DC and AT, the direct optical band gap energy, Egd, increases. All of these observation indicts that DT and AT significantly tunes the optical behaviors of ZSNP, making them promising candidates for optoelectronic applications.

Elucidating the Role of Carbon Impurities in Atomic-Scale Oxygen Precipitation Nucleation of Czochralski Silicon via Ab Initio Calculations

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In Czochralski-grown (Cz) silicon, bulk micro-defects (BMDs) incorporating oxygen precipitation serve as effective internal gettering sites and also help improve mechanical properties. As a common impurity in Cz silicon, carbon can be introduced either unintentionally or by doping. In this study, we employ ab initio calculations to elucidate how carbon impurities influence atomic-scale pathways of oxygen precipitation. Our results reveal that carbon atoms, depending on their lattice position, exhibit distinct behaviors that affect the migration and aggregation of oxygen species: Substitutional carbon is thermodynamically favored, while interstitial carbon shows high mobility and can form stable complexes with interstitial oxygen—most notably the C3 center. By systematically comparing the binding energies of various carbon- and vacancy-assisted oxygen agglomeration, we find that while carbon-related complexes can function as heterogeneous nucleation centers, their efficiency is limited compared with vacancies. This finding aligns well with experimental observations that only a high doping concentration of carbon can effectively enhance formation of oxygen precipitation and provides a theoretical perspective into the microscopic mechanism.

Multi-qubit DC gates over an inhomogeneous array of quantum dots

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The prospect of large-scale quantum computation with an integrated chip of spin qubits is imminent as technology improves. This invites us to think beyond the traditional 2-qubit-gate framework and consider a naturally supported ``instruction set'' of multi-qubit gates. In this work, we systematically study such a family of multi-qubit gates implementable over an array of quantum dots by DC evolution. A useful representation of the computational Hamiltonian is proposed for a dot-array with strong spin-orbit coupling effects, distinctive g-factor tensors and varying interdot couplings. Adopting a perturbative treatment, we model a multi-qubit DC gate by the first-order dynamics in the qubit frame and develop a detailed formalism for decomposing the resulting gate, estimating and optimizing the coherent gate errors with appropriate local phase shifts for arbitrary array connectivity. Examples of such multi-qubit gates and their applications in quantum error correction and quantum algorithms are also explored, demonstrating their potential advantage in accelerating complex tasks and reducing overall errors.