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PROCEEDINGS

Raman Spectroscopy and Modeling and Simulation of Quantum Dots and Nanomaterials for Optoelectronic and Sensing Applications

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ABSTRACT

Semiconducting quantum dots (Q-dots) with strain-tunable electronic properties are good contenders for quantum computing devices, as they hold promise to exhibit a high level of photon entanglement. The optical and electronic properties of Q-dots vary with their size, shape, and makeup. An assortment of Q-dots has been studied, including ZnO, ZnS, CdSe and perovskites [1]. We have employed both Raman spectroscopy (to precisely determine their vibrational frequencies) and UV-VIS spectroscopy (to determine accurately their band gap energies). The electronic band structure and density of states of the ZnO and ZnS Q-dots have been investigated under strain using Density Functional Theory (DFT). The computer program SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) was used to perform the DFT calculations via the linear combination of atomic orbitals (LCAO) method. The spin polarization of such systems may itself be used to encode information or influence the electronic properties of semiconducting Q-dots, which deserve special attention, as they have potential applications in lasers, photovoltaic cells, and imaging. In addition, we have investigated pristine and functionalized graphene nanoplatelets and metal oxides for sensing applications.

KEYWORDS

Raman spectroscopy; modeling; simulation; quantum dots; nanomaterials; optoelectronics; sensing

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References

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