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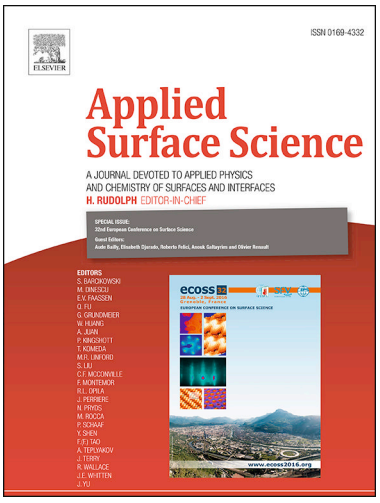

Full Length Article

GaAs monolayer: excellent SHG responses and semi metallic to metallic transition modulated by vacancy effect

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GaAs monolayer: excellent SHG responses and semi metallic to metallic transition modulated by vacancy effect

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Abstract

Monolayer materials are considered as a promising candidate for novel applications due to their attractive magnetic, electronic and optical properties. Investigation on nonlinear optical (NLO) properties and effect of vacancy on monolayer materials are vital to property modulations of monolayers and extending their applications. In this work, with the aid of first-principles calculations, the crystal structure, electronic, magnetic, and optical properties of GaAs monolayers with the vacancy were investigated. The result shows gallium arsenic (GaAs) monolayer produces a strong second harmonic generation (SHG) response. Meanwhile, the vacancy strongly affects structural, electronic, magnetic and optical properties of GaAs monolayers. Furthermore, arsenic vacancy (V_{As}) brings semi metallic to metallic transition, while gallium vacancy (V_{Ga}) causes nonmagnetic to magnetic conversion. Our result reveals that GaAs monolayer possesses application potentials in Nano-amplifying modulator and Nano-optoelectronic devices, and may provide useful guidance in designing new generation of Nano-electronic devices.

Key words

First-principles calculation; GaAs monolayer; SHG response; Vacancy

Introduction

The exploration of two-dimensional (2D) monolayer materials have received considerable attentions owing to their unique electronic, magnetic, and optical