

Effect of deformation on optical and optoelectronic properties of quasi-2D van der Waals heterostructures based on borophene

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The aim of this study

The aim of this study is to analyze the influence of uniaxial and biaxial tension/compression deformation on the optical and optoelectronic properties of borophene/ReS₂, borophene/GaN, and borophene/ZnO van der Waals heterostructures.

Methods and approaches

The van der Waals heterostructures were calculated by the DFT with PBE GGA implemented in the SIESTA 4.1.5 software package. The Grimme's correction scheme was used to describe the van der Waals interaction between heterostructure layers. To study the optical properties, the first order time dependent perturbation theory was used.

Conclusions

For the borophene/GaN, as the uniaxial compression increases, Im epsilon increases in the IR region. With increasing uniaxial stretching, an Im epsilon peak appears at the boundary of the visible and IR ranges and a peak in the IR range. In the case of biaxial deformation, a peak appears in the Im epsilon spectrum in the IR region when stretched by 6%. For the borophene/ZnO, in the case of uniaxial compression and in the case of uniaxial tension, an increase in Im epsilon in the IR region is observed with increasing deformation. The borophene/ReS₂ heterostructure turned out to be more sensitive to tension. In the case of biaxial deformation, both tension and compression noticeably affect the spectral profile of Im epsilon. For the borophene/ReSe₂ heterostructure, as the uniaxial compression increases, an increase in the Im epsilon values in the IR region is observed. With increasing uniaxial stretch, the Im epsilon peak at the boundary of the visible and IR ranges shifts to the IR region. When compressing heterostructures, the integral value of photocurrent in the solar IR spectrum increases. Stretching of heterostructures leads to the appearance of additional peaks of photocurrent and to an increase in their intensity.

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