Optoelectronic Properties of Van der Waals Heterostructures based on borophene, GaN, ZnO, $ReSe_2$ and ReS_2 monolayers

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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

It was revealed that 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 (~1300 nm). In the case of biaxial deformation, a peak appears in the Im epsilon spectrum in the IR region (~1100 nm) 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. In the case of biaxial deformation, no noticeable changes in the Im epsilon spectrum were observed. Of the two types of uniaxial deformations, 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. The value of Im epsilon within the IR range increases by 5-6 times compared to the undeformed structure. 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.

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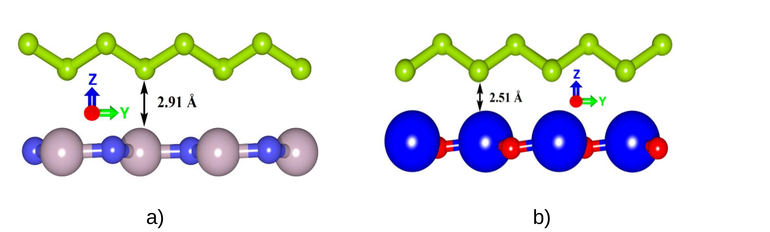
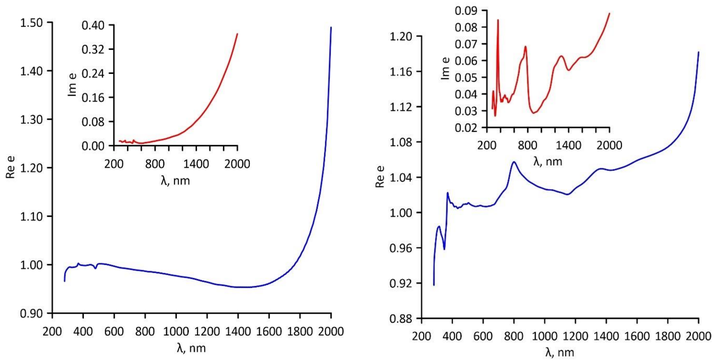


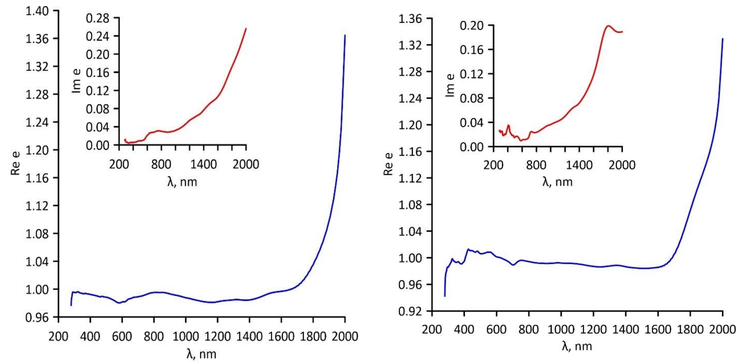
a) b)

Atomic structure of van der Waals heterostructures borophene/GaN (a) and borophene/ZnO (b)



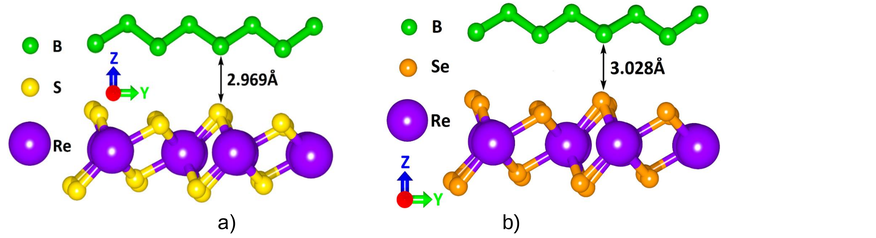
a) b)

Effect of uniaxial strain of 14% compression and tension on the complex dielectric constant of a borophene/GaN heterostructure



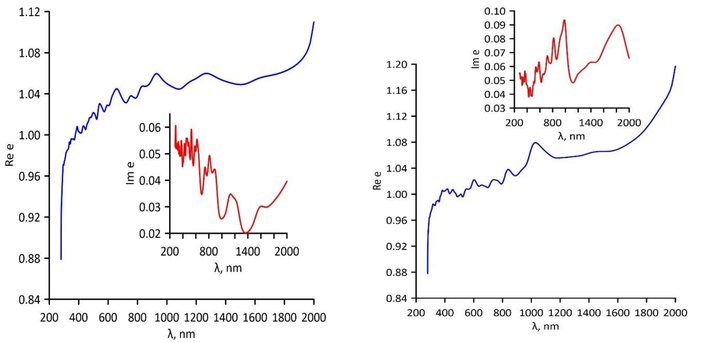
a) b)

Effect of uniaxial strain of 12% compression and tension on the complex dielectric constant of a borophene/ZnO heterostructure



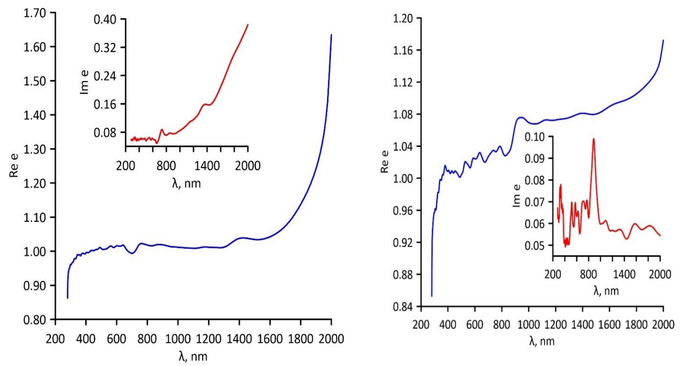
a) b)

Atomic structure of van der Waals heterostructures borophene/ReS2 (a) and borophene/ReSe2 (b)



a) b)

Effect of uniaxial strain of 12% compression and tension on the complex dielectric constant of a borophene/ReS2 heterostructure.



a) b)

Effect of uniaxial strain of 12% compression and tension on the complex dielectric constant of a borophene/ReSe2 heterostructure.