Rippling Effect on the Electrical Properties of Boron Nitride Monolayer: Density Functional Theory

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Received June 20, 2020
Revised September 4, 2020
Accepted for publication March 4, 2021

We performed a systematic study on mechanical properties of boron nitride monolayer. We found that applying mechanical deformation on boron nitride monolayer induced pattern of ripples. The induced rippling in the boron nitride monolayer created different bending levels in the forbidden zone, which in turn significantly tune the electronic properties of the monolayer. We also found that the band gap of boron nitride monolayer decreased dramatically with increasing the bending angles. In other words, the combined effect of applying bending and uniaxial stress on the boron nitride monolayer significantly decreases the band gap. We believe that the ability to precisely control sharp local curvatures of boron nitride sheet brings forward opportunities for strain-assisted modification of chemical reactivity and local electronic structure in the boron nitride monolayer. Such modification may be of great interest to band gap engineered devices.

Keywords: boron nitride monolayer, uniaxial stress, rippling, electrical properties, density functional theory.

Full text of the paper will appear in journal SEMICONDUCTORS.