Valence-force model and nanomechanics of single-layer phosphorene

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Abstract

In order to understand the relation of strain and material properties, both a microscopic model connecting a given strain to the displacement of atoms, and a macroscopic model relating applied stress to induced strain, are required. Starting from a valence-force model for black phosphorous (phosphorene) [1] we use recent experimental and computational results to obtain an improved set of valence-force parameters. From the model we calculate the phonon dispersion and the elastic properties of single-layer phosphorene [2]. Finally, we use these results to derive a complete continuum model, including the bending rigidities, valid for long-wavelength deformations of phosphorene. This continuum model is then used to study the properties of pressurized suspended phosphorene sheets.

References

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Figures

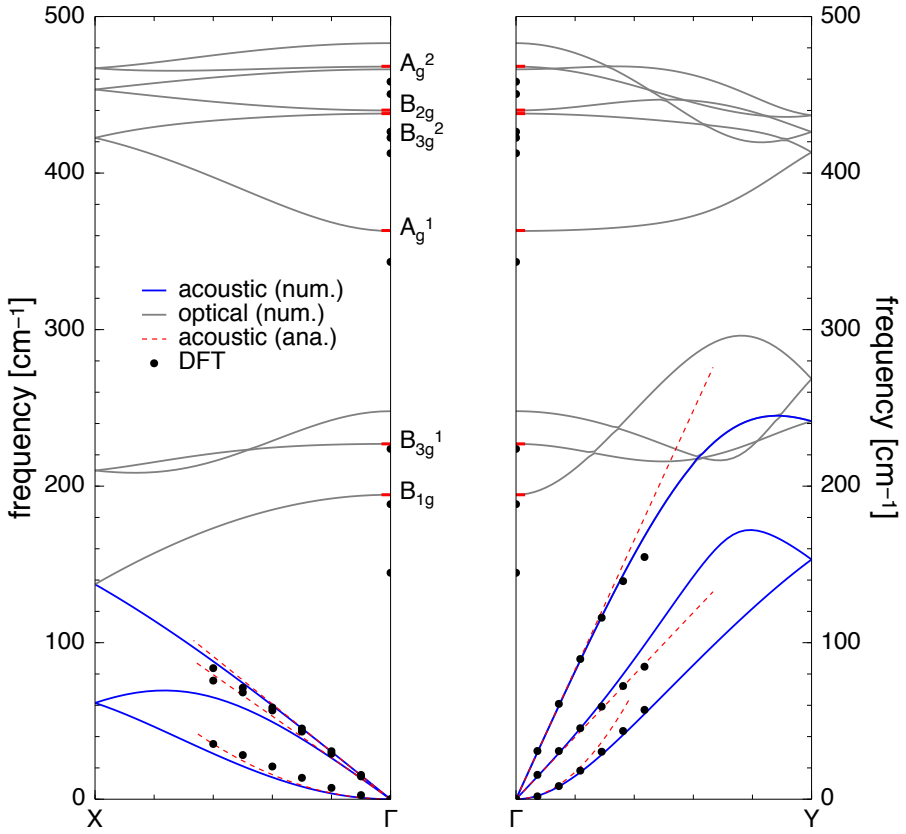

Figure: Phonon dispersion of phosphorene numerically calculated from the VFM is indicated by solid lines. The dashed lines show the behavior of the acoustic branches according to the continuum model. Filled circles are *ab initio* data from [3].