Electronic and Thermal Transport in Black Phosphorene tunned by Grain Boundaries and Strain.

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Grain Boundaries are a type of lattice defect that is common to find after the synthesis of 2D materials due to the growing and merging of two grains with different nuclear sites and lattice orientations. This type of defects influences the mechanical and electronic properties of the materials, therefore, with the understanding and control of this issue it is possible to engineer grain boundaries to tune transport properties of low dimensional systems.

In this work we used density functional based tight-binding (DFTB) method combined with atomistic Green Functions technique to calculate the transport properties. We show the electronic and phonon transport properties of two grain boundaries types in Black Phosphorene. Additionally, we included strain as additional parameter to tune their transport properties.

References

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