

Abstract Submitted
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Phase Transition between Black and Blue Phosphorenes: A Quantum Monte Carlo Study LESHENG LI, YI YAO, KYLE REEVES, YOSUKE KANAI, Univ of NC - Chapel Hill — Phase transition of the more common black phosphorene to blue phosphorene is of great interest because they are predicted to exhibit unique electronic and optical properties[1]. However, these two phases are predicted to be separated by a rather large energy barrier. In this work, we study the transition pathway between black and blue phosphorenes by using the variable cell nudge elastic band method combined with density functional theory calculation. We show how diffusion quantum Monte Carlo method can be used for determining the energetics of the phase transition and demonstrate the use of two approaches for removing finite-size errors. Finally, we predict how applied stress can be used to control the energetic balance between these two different phases of phosphorene. [1] Zhu, Zhen, and David Tománek. "Semiconducting layered blue phosphorus: A computational study." *Physical review letters* 112.17 (2014): 176802.

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