Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Phase Transitions of Bulk Black Phosphorus and Few-Layer Phosphorene from First Principles[1] KEIAN NOORI, Centre for Advanced 2D Materials, National University of Singapore, SU YING QUEK, Centre for Advanced 2D Materials Department of Physics, National University of Singapore — Bulk black phosphorus (BP) undergoes phase transitions under pressure, transitioning from the orthorhombic to the rhombohedral (A-7) phase at 40-80 kbar [1], and from the A-7 to the simple cubic phase at ca. 110 kbar [1], the latter being superconducting. Phosphorene, a monolayer of the orthorhombic phase of BP, demonstrates many attractive characteristics, including high carrier mobility, high optical and UV absorption, and anisotropic mechanical, electronic, optical, and transport properties [2]. The pressure-induced phase transitions of few-layer phosphorene, however, have not yet been thoroughly studied, and it remains unclear if and at what pressures it transitions to the corresponding rhombohedral and simple cubic phases. In this work we study the pressure-induced phase transitions of bulk BP and few-layer phosphorene from first-principles density functional theory calculations, exploring the complex effects of different exchange-correlation functionals and finite temperature.
[1] J. C. Jamieson, Science 139, 1291 (1963); T. Kikegawa and H. Iwasaki, Acta. Cryst. B39, 158 (1983); H. Kawamura, et al. Solid State. Commun. 49, 879 (1983)
[2] A. Carvalho, et al., Nat. Rev. Mater. 1, 16061 (2016)

[1]We acknowledge support from the Singapore National Research Foundation, Prime Ministers Office, under its medium-sized centre program and under grant NRF-NRFF2013-07.

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Date submitted: 10 Nov 2016 Electronic form version 1.4