Abstract Submitted
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Twisted Phosphorene Nanoribbons WOOSUN JANG, KISUNG KANG, ALOYSIUS SOON, Department of Materials Science and Engineering, Yonsei University — Many different forms of structural deformations have been employed to alter the electronic structure of various two-dimensional (2D) nanomaterials in various optoelectronic devices [1]. Given the recent interest in the new class of 2D nanomaterials – phosphorene, it is important to understand how the anisotropic strain-dependent electronic properties of low-dimensional phosphorene may be exploited for technological gain. Here, using first-principles density-functional theory, we investigate the mechanical stability of twisted one-dimensional phosphorene nanoribbons (PNR) by measuring its critical twist angle (θ_c) and shear modulus as a function of the applied mechanical torque [2-4]. We find a strong anisotropic behaviour in PNRs with different edge terminations and directions, and report the direct consequence of this applied mechanical stress on its corresponding electronic (and optical) properties. [1] E. S. Reich, *Nature*, **506**, 19 (2014); [2] C. D. Reddy *et al., Appl. Phys. Lett.* **94**, 101904 (2009); [3] E. M. Diniz, *Appl. Phys. Lett.* **104**, 083119 (2014); [4] V. Sorkin and Y. Zhang, *Nanotechnology*, **26**, 235707 (2015)

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