

Abstract Submitted  
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**Ground state degeneracy, energy barriers, and molecular dynamics evidence for two-dimensional disorder in black phosphorus and monochalcogenide monolayers at finite temperature** MEHRSHAD MEHBOUDI, SALVADOR BARRAZA-LOPEZ, ALEX M. DORIO, University of Arkansas, WENJUAN ZHU, AREND VAN DER ZANDE, University of Illinois, HUGH O. H. CHURCHILL, University of Arkansas, ALEJANDRO A. PACHECO-SANJUAN, Universidad del Norte, EDMUND O. HARRISS, PRADEEP KUMAR, University of Arkansas — Mono-layers of black phosphorus and other two dimensional materials such as mono-layers of SiSe, GeS, GeSe, GeTe, Sns, SnSe, and SnTe with a similar crystalline structure have a four-fold degenerate ground state that leads to two-dimensional disorder at finite temperature. Disorder happens when neighboring atoms gently re-accommodate bonds beyond a critical temperature. In this talk, the effect of atomic numbers on the transition temperature will be discussed. In addition Car-Parinello molecular dynamics calculations at temperatures 30, 300 and 1000 K were performed on supercells containing more than five hundred atoms and the results from these calculations confirm the transition onto a two-dimensional disordered structure past the critical temperature, which is close to room temperature for many of these compounds. References: M. Mehboudi, A.M. Dorio, W. Zhu, A. van der Zande, H.O.H. Churchill, A.A. Pacheco Sanjuan, E.O.H. Harris, P. Kumar, and S. Barraza-Lopez. arXiv:1510.09153.

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