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Prediction of a strain-tunable 2D Topological Dirac semimetal in monolayers of black phosphorus XIUWEN ZHANG, QIHANG LIU, ALEX ZUNGER, University of Colorado, Boulder, THEORY TEAM — N-dimensional Topological Nonmetals (TNM) such as N = 2D HgTe/CdTe quantum wells or N = 3D Bi_2Se_3 have a finite (often tiny) band gap between occupied and unoccupied bands, and show conductive Dirac cones in their N-1 dimensional geometric boundaries. On the other hand, examples of topological semimetals (TSM) are known for 3D solids (Cd_3As_2) where they have Dirac cones in the 3D system itself. Using density functional calculation of bands and the topological invariant Z_2 we predict the existence of 2D topological Dirac semimetal in few monolayers of strain tuned black phosphorus (BP), with Dirac cones induced by band inversion. The band structures of few monolayers and bulk crystal of BP under a few percent biaxial and uniaxial strains were calculated using state-of-art electronic structure methods. The critical strain of the transition to TSM was found to decrease as the layer thickness increases. We will discuss the protection of the Dirac cones by the crystalline symmetry in the 2D TSM and the manipulation of crystalline symmetry, which induces further topological phase transitions. Supported by the NSF-DMREF-13-34170.

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