Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

**Extraordinary Bending Effects in MoS2, Phosphorene, and Graphene Nanoribbons**[1] LIPING YU, ADRIENN RUZSINSZKY, JOHN PERDEW, Temple University — The two-dimensional (2D) materials show great potential for flexible electronics and energy applications. They have remarkable mechanical, electronic, thermal and optical properties, which are often coupled to each other. In this talk, we shall present our first principles study on the bending effects in the electronic structure of $MoS_2$, phosphorene, and graphene nanoribbons. We predict that mechanical bending, as a unique attribute of thin 2D materials, can be used to control conductivity and Fermi-level shift. We find that bending can control the charge localization of top valence bands in both $MoS_2$ and phosphorene nanoribbons. The donor-like in-gap edge-states of armchair $MoS_2$ ribbon and their associated Fermi-level pinning can be removed by bending. A bending-controllable new in-gap state and accompanying direct-indirect gap transition are predicted in armchair phosphorene nanoribbon. We demonstrate that such emergent bending effects are realizable in experiment and can be attributed to the highly non-uniform and enormously large local in-plane strains induced by bending. The bending stiffness as wells as the effective thickness of 2D materials are also derived from first principles.

[1]The work was supported as part of the Center for the Computational Design of Functional Layered Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science

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Date submitted: 06 Nov 2015 Electronic form version 1.4