Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Tiling Phosphorene[1] ZHEN ZHU, DAVID TOMANEK, JIE GUAN, Michigan State University — We introduce a scheme to categorize the structure of different layered phosphorene allotropes by mapping their non-planar atomic structure onto a two-color 2D triangular tiling pattern. In the puckered structure of a phosphorene monolayer, we assign atoms in "top" positions to dark tiles and atoms in "bottom" positions to light tiles. Optimum sp^3 bonding is maintained throughout the structure when each triangular tile is surrounded by the same number N of like-colored tiles, with $0 \leq N \leq 2$. Our *ab initio* density functional calculations indicate that both the relative stability and electronic properties depend primarily on the structural index N. The proposed mapping approach may also be applied to phosphorene structures with non-hexagonal rings and 2D quasicrystals with no translational symmetry, which we predict to be nearly as stable as the hexagonal network.

[1]Supported by the National Science Foundation Cooperative Agreement #EEC-0832785, titled "NSEC: Center for High-rate Nanomanufacturing".

Zhen Zhu
Michigan State University

Date submitted: 02 Nov 2014 Electronic form version 1.4