Tiling Phosphorene\textsuperscript{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 \textit{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.

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