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High stability of faceted nanotubes and fullerenes of multi-phase layered phosphorus: A computational study[1] JIE GUAN, ZHEN ZHU, DAVID TOMANEK, Michigan State University — We present a paradigm in constructing very stable, faceted nanotube and fullerene structures by laterally joining nanoribbons or patches of different planar phosphorene phases. Our *ab initio* density functional calculations indicate that these phases may form very stable, non-planar joints. Unlike fullerenes and nanotubes obtained by deforming a single-phase planar monolayer at substantial energy penalty, we find faceted fullerenes and nanotubes to be nearly as stable as the planar single-phase monolayers. The resulting rich variety of polymorphs allows to tune the electronic properties of phosphorene nanotubes (PNTs) and fullerenes not only by the chiral index, but also by the combination of different phosphorene phases. In selected PNTs, a metal-insulator transition may be induced by strain or changing the number of walls.

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