Abstract Submitted
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Unusually stable helical coil allotrope of phosphorus[1] DAVID TOMANEK, DAN LIU, JIE GUAN, Michigan State University, JINGWEI JIANG, Peking University — We have identified an unusually stable helical coil allotrope of phosphorus. Our *ab initio* density functional theory calculations indicate that the uncoiled, isolated straight 1D chain is equally stable as a monolayer of black phosphorus dubbed phosphorene. The coiling tendency and the attraction between adjacent coil segments add an extra stabilization energy of ≈12 meV/atom to the coil allotrope, similar in value to the ≈16 meV/atom inter-layer attraction in bulk black phosphorus. Thus, the helical coil structure is essentially as stable as black phosphorus, the most stable phosphorus allotrope known to date, and has a direct fundamental band gap similar to that of phosphorene monolayer structures. With an optimum radius of 2.4 nm, the helical coil of phosphorus may fit well and even form inside wide carbon nanotubes.

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