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Light element based low dimensional compounds with penta-structure SHUNHONG ZHANG, Institute for Advanced Study, Tsinghua University; Center for Applied Physics and Technology, Peking University, XIAOYIN LI, Center for Applied Physics and Technology, Peking University, JIAN ZHOU, Department of Physics, Virginia Commonwealth University, QIAN WANG, Center for Applied Physics and Technology, Peking University, PURU JENA, Department of Physics, Virginia Commonwealth University — Previously we proposed penta-graphene (PG) as a two dimensional carbon structure that is only composed of carbon pentagons. Its novel properties such as negative Poisson's ratio have raised broad interest. Inspired by this study many PG-like light element based low dimensional compounds have been theoretically designed via first principles calculations. Here we present some of such examples. The first one is penta-CN₂, a chemical analogue of PG, which is characterized by its unexpected high nitrogen content and high in-plane stiffness. It also exhibits an interesting nonsymmorphic symmetry protected band degeneracy at the Brillouin zone edge. We also investigate the chemical derivatives of PG obtained via hydrogenation and halogenation. Such surface functionalization can effectively tune the electronic, mechanical and thermal properties of PG. Finally, we will briefly introduce experimental progress of realization of low dimensional penta-structures.

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