Abstract Submitted
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A Pentagon Based Carbon Sheet QIAN WANG, SHUNHONG ZHANG[1], Center for Applied Physics and Technology, Peking University, JIAN ZHOU, Physics Department, Virginia Commonwealth University, XIAOSHUANG CHEN, Shanghai Institute of Technical Physics, Chinese Academy of Science, YOSHIYUKI KAWAZOE, Institute for Material Research, Tohoku University, Japan, PURU JENA, Physics Department, Virginia Commonwealth University, A INTERNATIONAL TEAM COLLABORATION — A new two-dimensional (2D) meta-stable carbon allotrope, penta-graphene, composed entirely of carbon pentagons and resembling the Cairo pentagonal tiling, is proposed. State-of-the-art theoretical calculations confirm that the new carbon polymorph is not only dynamically and mechanically stable, but also can withstand temperatures as high as 1000 K. Due to its unique atomic configuration penta-graphene has an unusual negative Poisson's ratio (NPR) and ultra-high ideal strength that can even outperform graphene. Furthermore, unlike graphene that needs to be functionalized for opening a band gap, penta-graphene possesses an intrinsic quasi-direct band gap as large as 3.25 eV - close to that of ZnO and GaN. Equally important, when rolled up, penta-graphene can form a pentagon-based nanotube. The resulting penta-carbon nanotubes are semiconducting regardless of their chirality. When stacked in different patterns, dynamically and thermally stable 3D twin structures of T12-carbon are generated with band gaps even larger than that of T12-carbon. The versatility of penta-graphene and its derivatives are expected to have broad applications in nanoelectronics and nanomechanics.

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