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Phosphorenes with Non-Honeycomb Structures: A Much Extended Family[1] MENGHAO WU, HUAHUA FU, Huazhong University of Science and Technology, LING ZHOU, Miami University, KAILUN YAO, Huazhong University of Science and Technology, XIAO CHENG ZENG, University of Nebraska-Lincoln, HUAZHONG UNIVERSITY OF SCIENCE AND TECHNOLOGY TEAM, UNIVERSITY OF NEBRASKA-LINCOLN TEAM — We predict a new class of monolayer phosphorous allotropes, namely, ε-P, ζ-P, η-P and θ-P. Distinctly different from the monolayer α-P (black) and previously predicted β-P (Phys. Rev. Lett. **112**, 176802 (2014)), γ-P and δ-P (Phys. Rev. Lett. **113**, 046804 (2014)) with buckled honeycomb lattice, the new allotropes are composed of P_4 square or P_5 pentagon units that favor tricoordination for P atoms. The new four phases, together with 5 hybrid phases, are confirmed stable by first-principles calculations. In particularly, the θ-P is shown to be equally stable as the α-P (black) and more stable than all previously reported phosphorene allotropes. Prediction of nonvolatile ferroelastic switching and structural transformation among different phases under strains points out their potential applications via strain engineering.

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