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Chemical scissors cut phosphorene and their novel electronic properties XIHONG PENG, Arizona State University, QUN WEI, Arizona State University, Xidian University — Phosphorene, a recently fabricated two-dimensional puckered honeycomb structure of black phosphorus, showed promising properties for applications in nano-electronics. In this work, we report a chemical scissors effect on phosphorene, using first principles density-functional methods. It was found that chemical species, such as H, OH, F, and Cl, can act as scissors to cut phosphorene. Phosphorus nanochains and nanoribbons can be obtained using such chemical scissors. The scissors effect results from the strong bonding between the chemical species and phosphorus atoms. Other species such as O, S and Se fail to cut phosphorene due to their weak bonding with phosphorus. The electronic structures of the produced P-chains reveal that the hydrogenated P-chain is an insulator; however, the pristine P-chain is a one-dimensional Dirac material, in which the charge carriers are massless fermions travelling at an effective speed of light approximately 8×10^5 m/s. The obtained zigzag phosphorene nanoribbons show either metallic or semiconducting behaviors, depending on the treatment of the edge phosphorus atoms.

[1] X.-H. Peng, Q. Wei, "Chemical scissors cut phosphorene nanostructures," Material Research Express, in press.

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