

VIOLET PHOSPHORUS AND PHOSPHORENE

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Black phosphorene has attracted much attention as a semiconducting two - dimensional material. Violet phosphorus is another layered semiconducting phosphorus allotrope with unique electronic and optoelectronic properties. However, no confirmed violet crystals or reliable lattice structure of violet phosphorus had been obtained. Now, violet phosphorus single crystals were produced and the lattice structure has been obtained by single - crystal *x* - ray diffraction to be monoclinic with space group of P2/n (13) (*a*=9.210 Å, *b*=9.128 Å, *c*=21.893 Å, β =97.776°). The lattice structure obtained was confirmed to be reliable and stable. The optical band gap of violet phosphorus is around 1.7 eV, which is slightly larger than the calculated value. The thermal decomposition temperature was 52 °C higher than its black phosphorus counterpart, which was assumed to be the most stable form. Violet phosphorene was easily obtained by both mechanical and solution exfoliation under ambient conditions.



Figure 1. The crystal structure of violet phosphorus. (a) Minimum asymmetric unit; (b) Optical microscope image of a violet phosphorus single crystal; The phonon dispersive curves of violet phosphorus (c) from 1969 and (d) our violet phosphorus in the Brillouin zone.