

Supporting Information for:

Changing the Phosphorus Allotrope from a Square Columnar Structure to a Planar Zigzag Nanoribbon by Increasing the Diameter of Carbon Nanotube Nanoreactors

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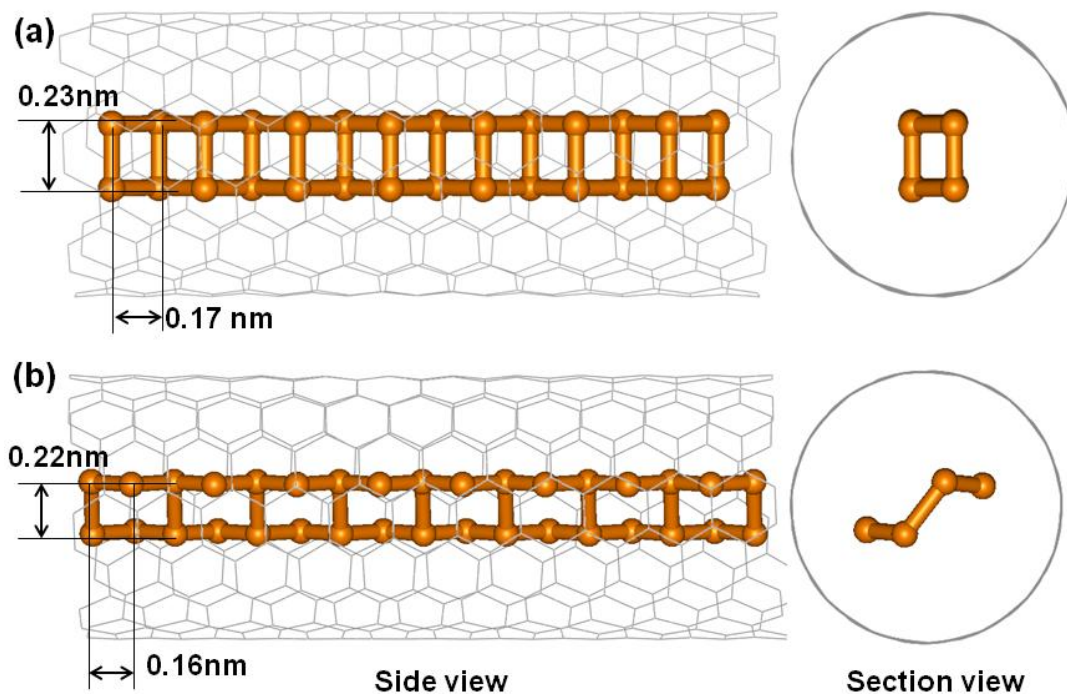


Figure S1. Structural models of (a) AR-P@SWCNT and (b) AR-P@SWCNT.

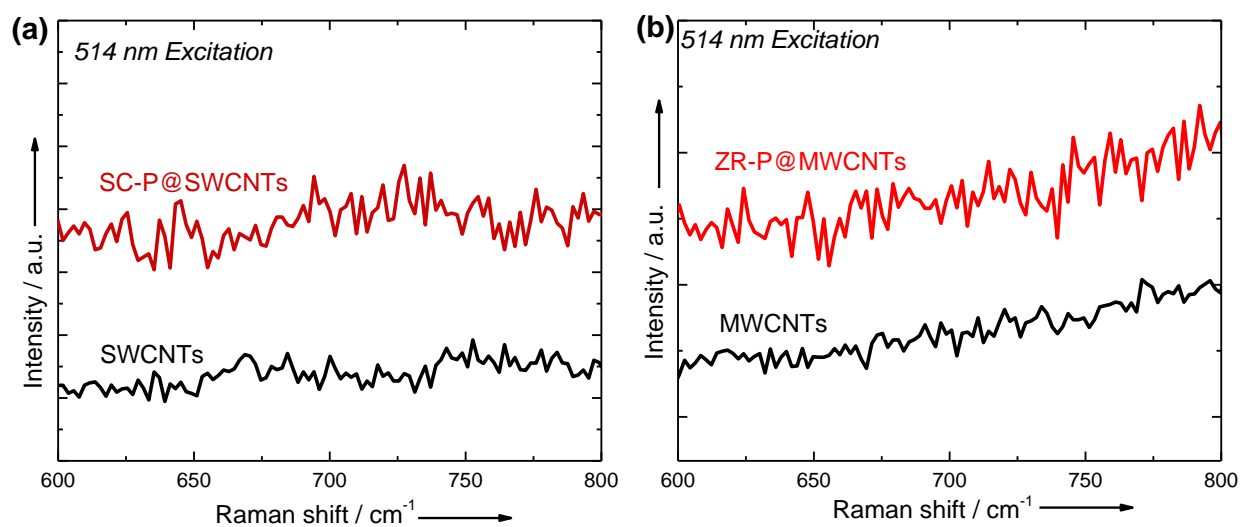


Figure S2. Raman spectra of pristine and phosphorus-filled (a) SWCNTs and (b) MWCNTs. Spectra of pristine nanotubes are shown in black and those of P-filled nanotubes in red.

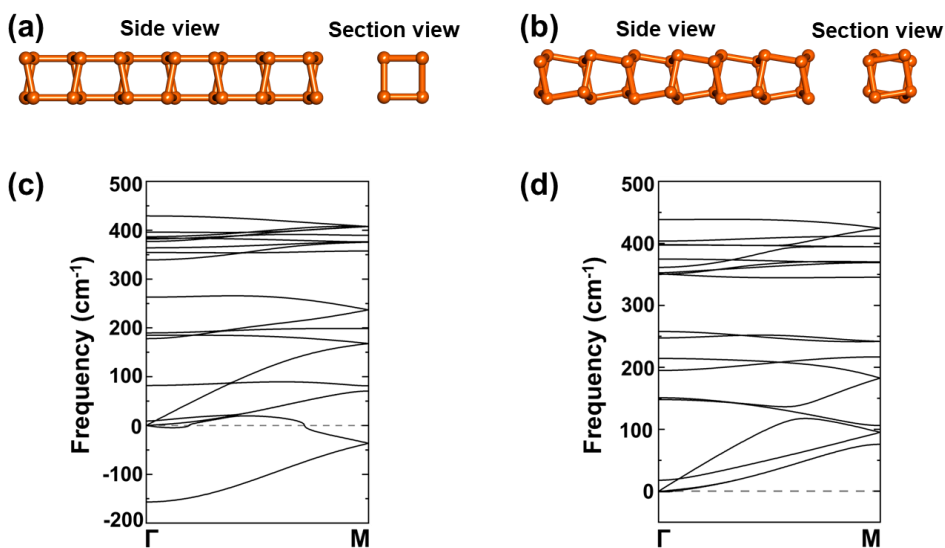


Figure S3. (a, b) structural model and (c, d) vibrational phonon spectra of unstable straight (left) and stable twisted (right) SC-P structures.

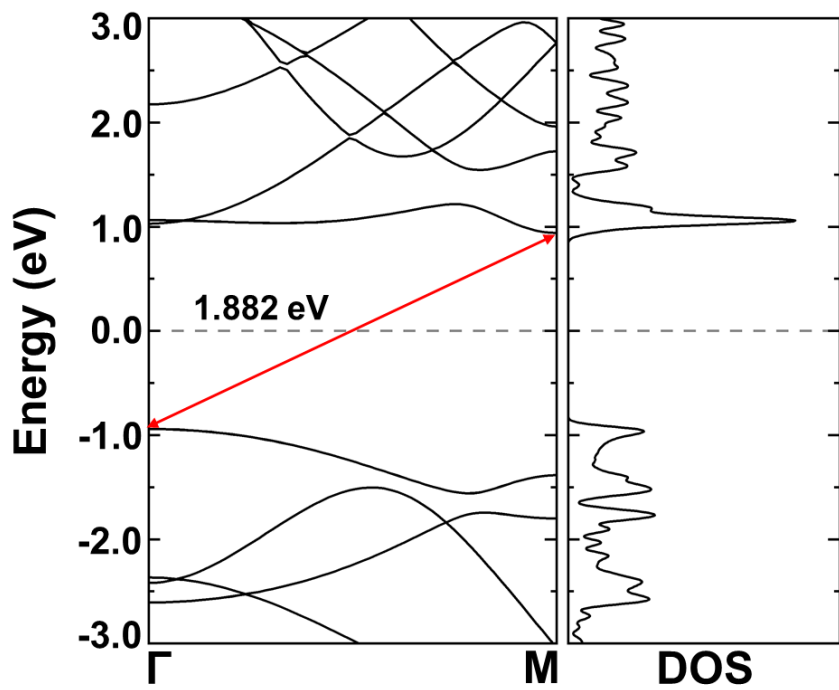


Figure S4. Electronic band structure and density of states (DOS) for the twisted SC-P allotrope based on DFT-PBE calculations. An indirect band gap is indicated by the red arrow.