Encapsulated phosphorus packings in Single-Walled Carbon Nanotube: A Raman Spectroscopy investigation

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Abstract

Elemental phosphorus P displays an enormous number of allotropes with highly different physical and chemical properties [1]. Previous experimental works showed how the encapsulated tetra-phosphorus P_4 molecules into single-walled carbon nanotubes (SWCNTs) opened the route to investigate highly reactive intermediate phases from white to red P [2]. The inserted red phosphorus into carbon nanotubes displays a novel arrangement into not-well known interacting tubular structures of P_{12} and P_{14} nanorods. The encapsulated P allotropes are visualized by transmission electron microscopy and their covalent substructures were unravelled via Raman spectroscopy [3]. The prediction of hierarchical scale among all possible phosphorus chains was investigated by dispersive-corrected density functional theory (DFT). The Raman intensities of most promising candidates of P allotropes were determined computationally by using the semi-classical Placzek approximation [3]. The current experimental work joint with computational support provides strong evidences on the fascinating structural diversity of phosphorus and the discovery of new modifications due to the charge transfer with SWCNTs.

References

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Figures

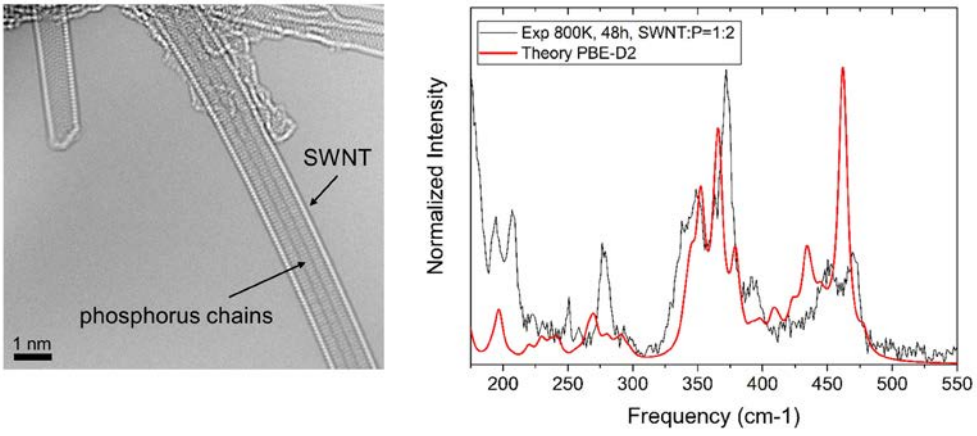

Figure 1: (Left) Transmission electron microscopy image of encapsulated phosphorus allotropes inside SWCNT. (Right) Comparative Raman spectrum between experimental (black line) and corresponding theoretical (red line) counterpart.