Starfish-like phosphorus carbide nanotubes

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Recently several allotropes of a novel two-dimensional material, phosphorus carbide (PC), have been predicted theoretically and some of them have already been successfully fabricated [1]. For one of these PC allotropes, α-PC, the possibility of its rolling to a PC nanotube (PCNT) at room temperature under compressive strain has been found [2]. These PCNTs of different sizes exhibit high thermal stability and possess well tunable band gap. In this work, PCNT obtained by the rippling of β_0-PC and β_1-PC monolayers along their armchair (APCNT) and zigzag (ZPCNT) directions are investigated in the framework of density functional theory.

It has been found that most of created β-PCNTs possess starfish-like structure (see Figure 1a). The dynamical stability of these β-PCNTs has been verified using *ab initio* molecular dynamics calculations conducted at 300 K. It is also found that β-PCNTs of the smallest/biggest size consist of 12/44 atoms. According to electronic band structure calculations, β-PCNTs can be semiconductors, semimetals or metals depending on their size and form (see Figure 1b). Therefore, due to their extraordinary form and highly tunable band structure, β-PCNTs may find the application in straintronic, optical and photovoltaic devices.

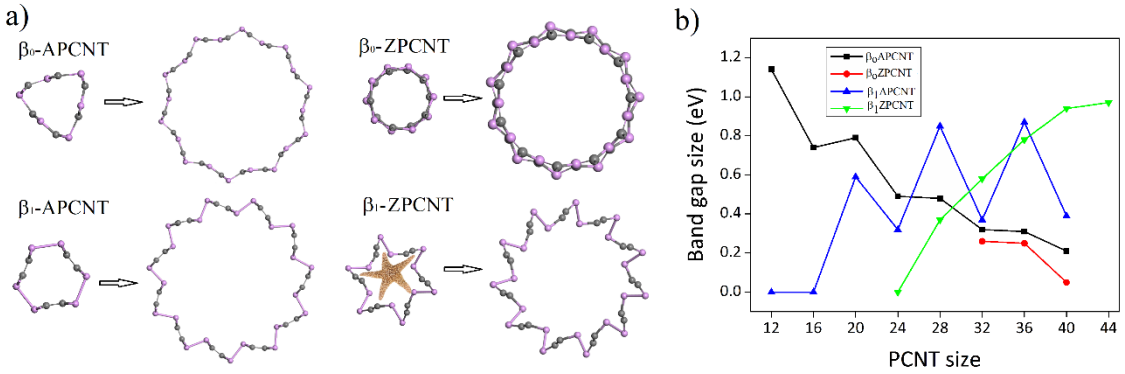

Figure 1. (a) Atomic structure and (b) band gap size as a function of size of β_0- and β_1-APCNT and β_0- and β_1-ZPCNT.

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