Supplementary Article

Acetylenic linkage dependent electronic and optical behaviour of morphologically distinct `-ynes’

Susmita Jana, Arka Bandyopadhyay, Debnarayan Jana*

Department of Physics, University of Calcutta, 92 Acharya Prafulla Chandra Road, Kolkata 700009, India.

* Corresponding Author. E-mail Address: djphy@caluniv.ac.in, Fax: 0091 033 2350 9755.
Figure 1: Phonon spectra for the entire Brillouin zone for (a) $\alpha$-T graphyne, (b) $\beta$-T graphyne, (c) T-graphdiyne and (d) T-graphtriyne.
Figure 2: AIMD (ab initio molecular dynamics) simulation for (a) $\alpha$-T graphyne, (b) $\beta$-T graphyne, (c) T-graphdiyne and (d) T-graphtriyne at 1500 K with the timestep of 1fs.
Figure 3: Electronic band spectra calculated from DFT for (a) α-T graphyne, (b) β-T graphyne, (c) T graphene, (d) γ-T graphyne, (e) T graphdiyne, (f) T graphtriyne.
Figure 4: Electronic band spectra calculated from TB analysis for (a) T graphene, (b) γ-T graphyne, (c) β-T graphyne, (d) T graphdiyne.
Figure 5: Reflectivity coefficient variation with energy.