

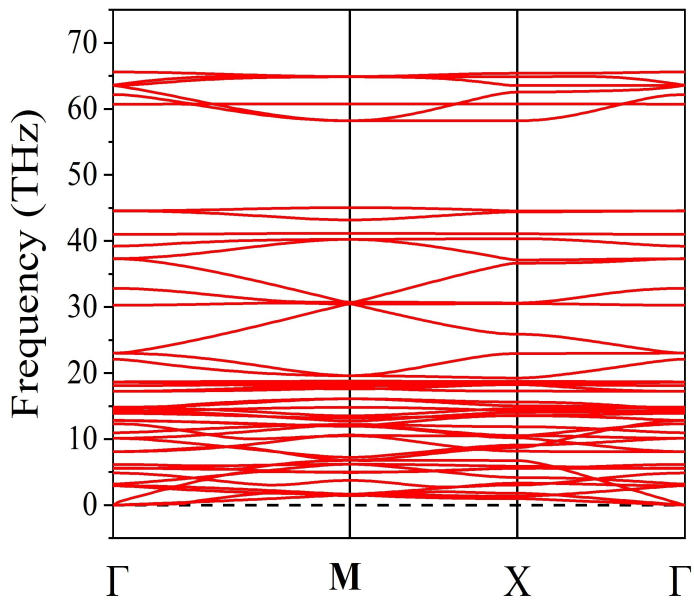
Supplementary Article

**Acetylenic linkage dependent electronic and  
optical behaviour of morphologically distinct '-ynes'**

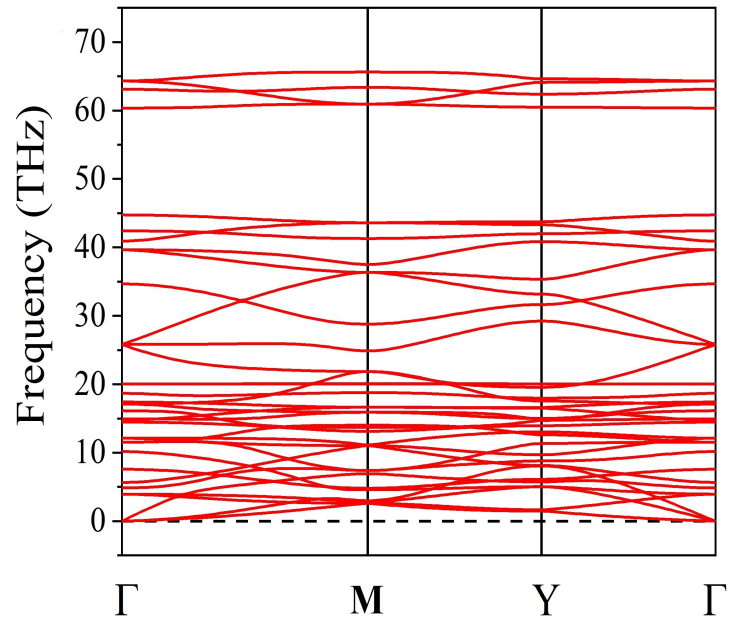
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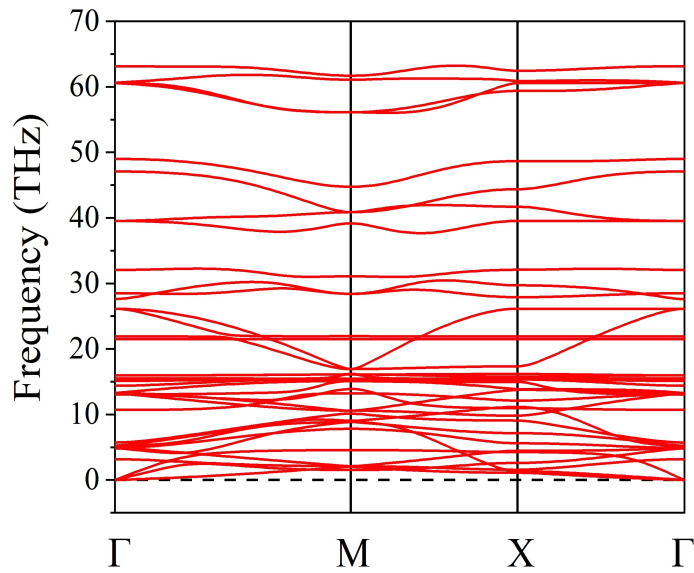
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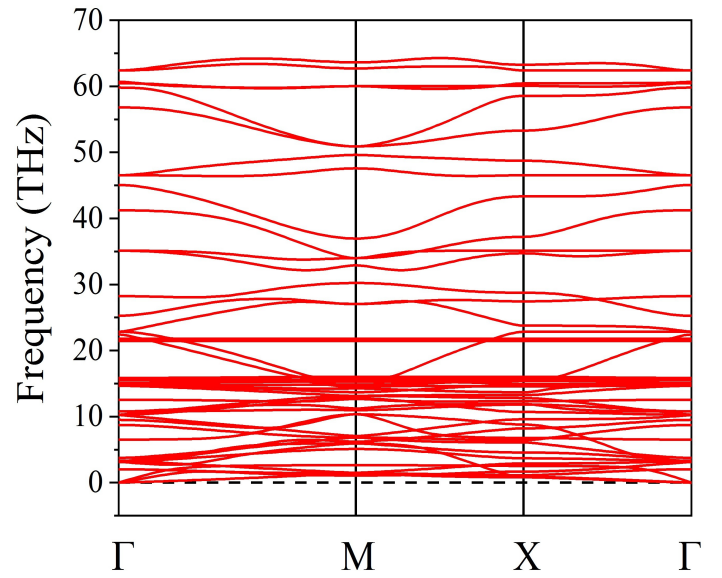
(a)



(b)

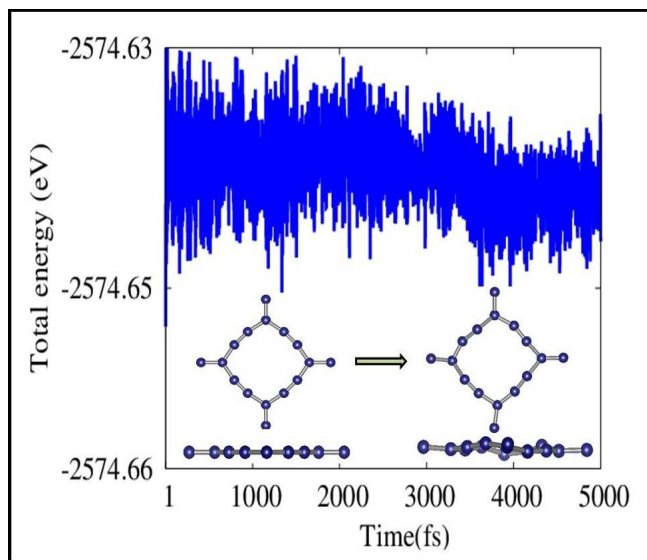


(c)

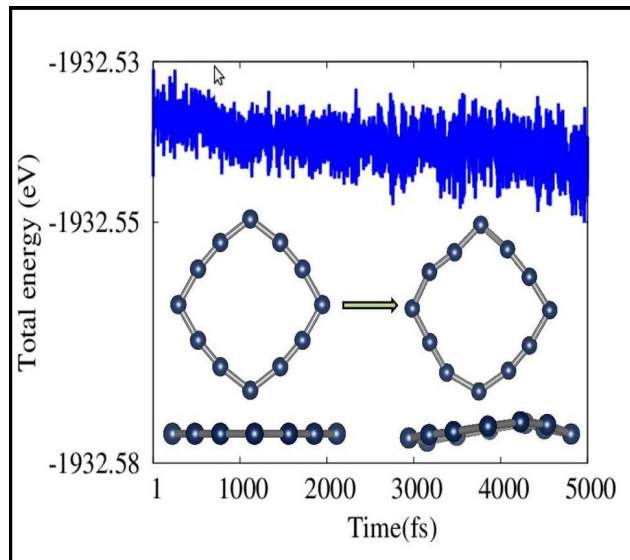


(d)

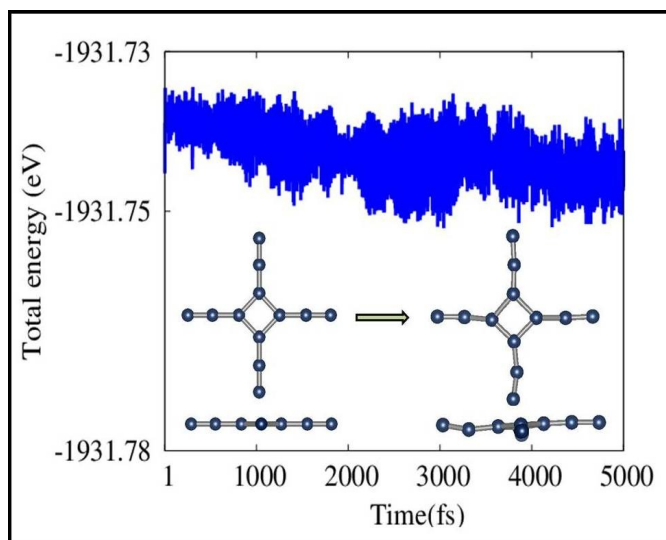
**Figure 1 : Phonon spectra for the entire Brillouin zone for (a)  $\alpha$ -T graphyne, (b)  $\beta$ -T graphyne, (c) T-graphdiyne and (d) T-graphtriyne.**



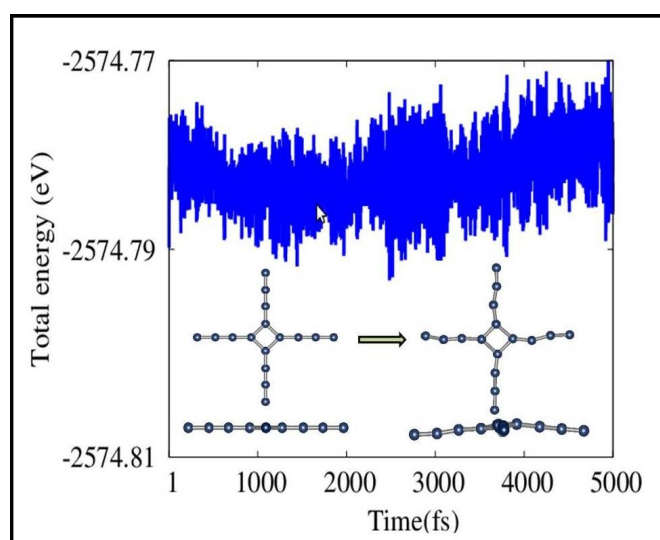
(a)



(b)

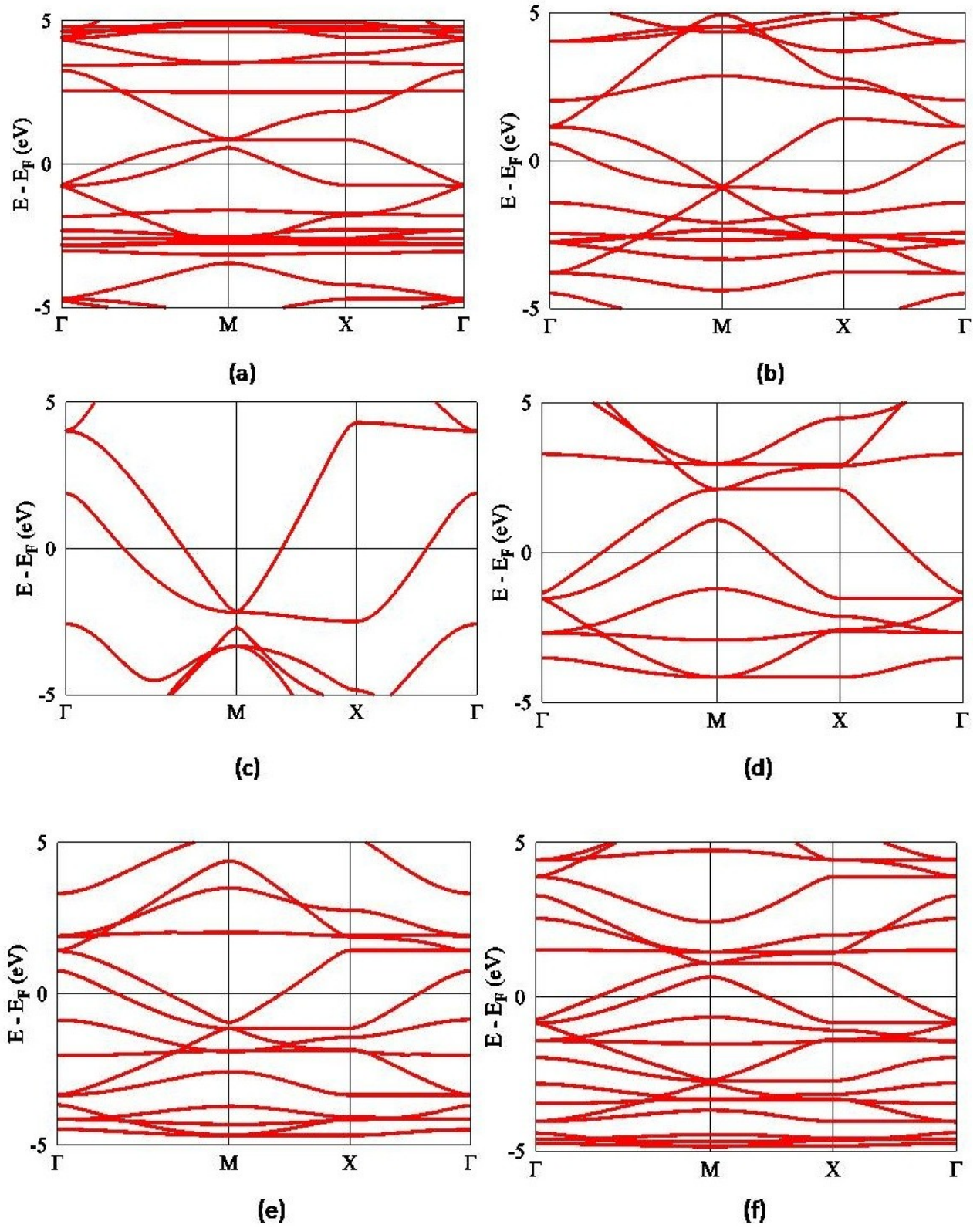


(c)



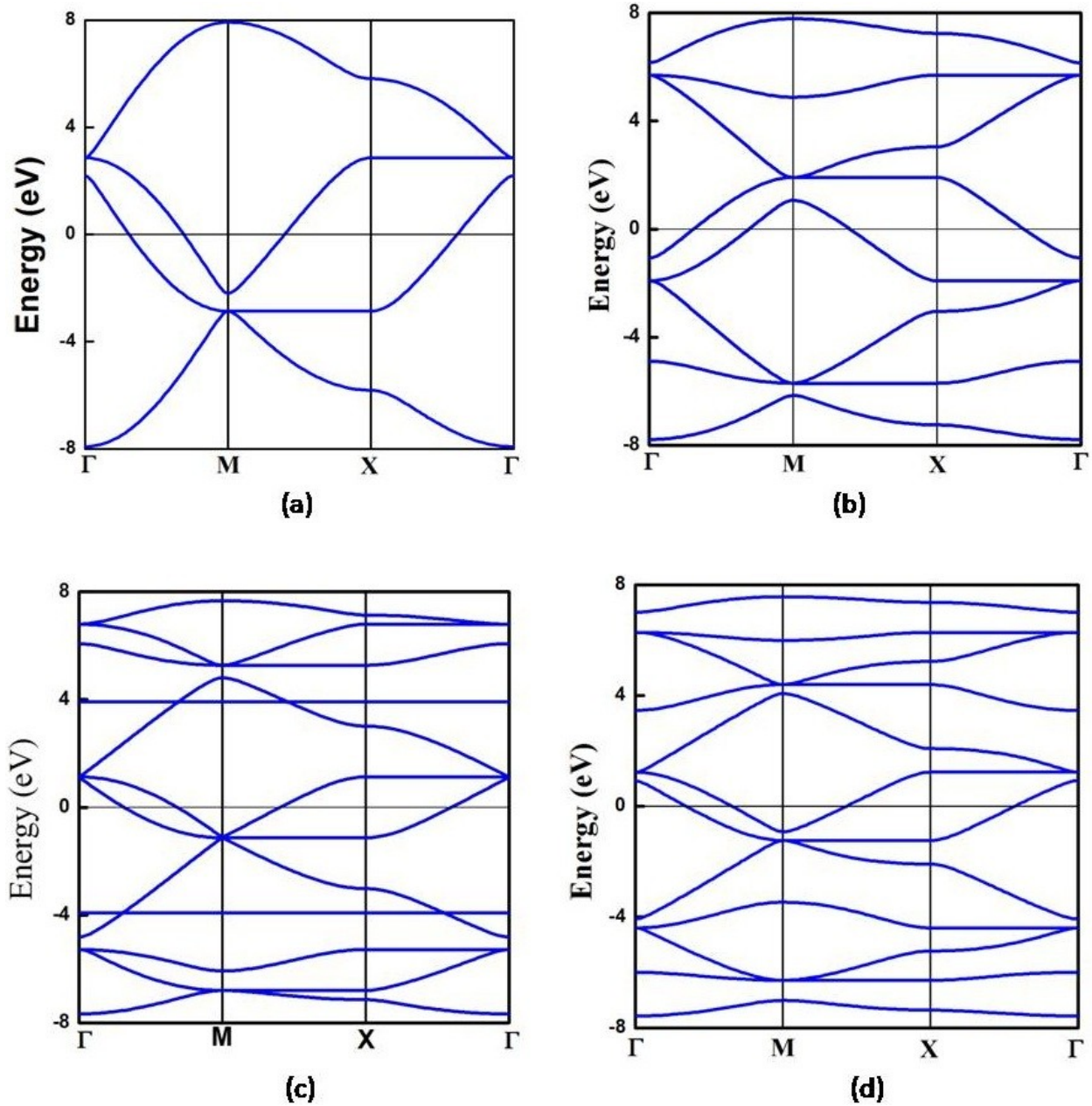
(d)

**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)  $\alpha$ -T graphyne , (b)  $\beta$ -T graphyne ,(c) T graphene, (d)  $\gamma$ -T graphyne, (e) T graphdiyne, (f) T graphtriyne.**





**Figure 4:** Electronic band spectra calculated from TB analysis for (a) T graphene, (b)  $\gamma$ -T graphyne, (c)  $\beta$ -T graphyne, (d) T graphdiyne.

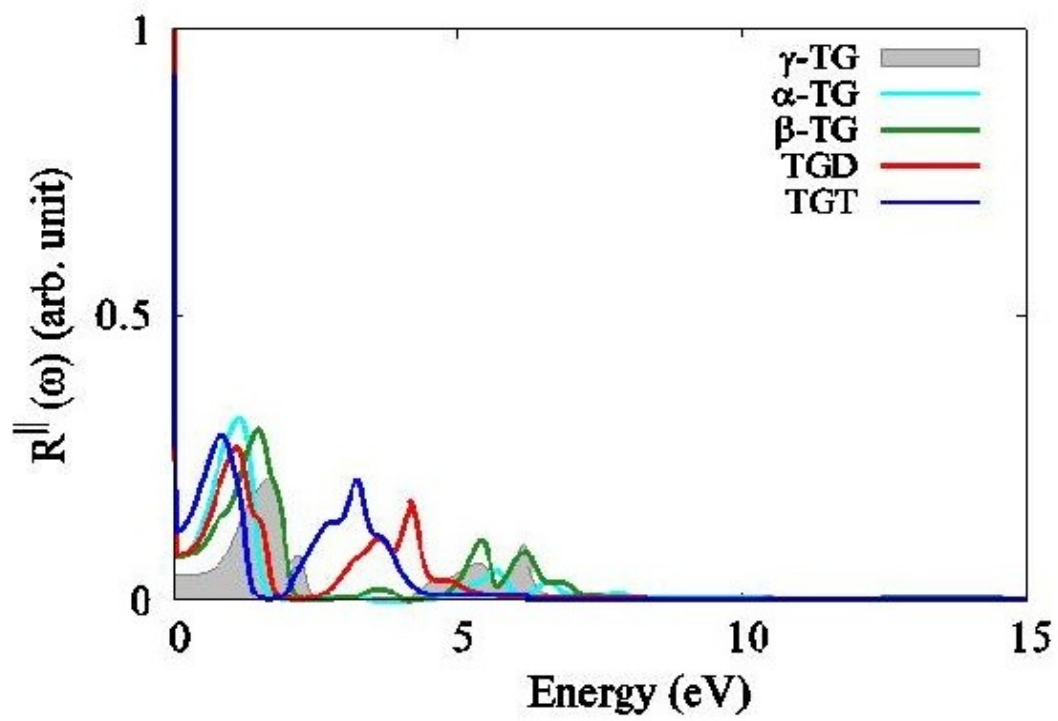


Figure 5 : Reflectivity co-efficient variation with energy.