**Abstract**

Since the discovery of CNT by Iijima, Nature 354, 56 (1991). CNT’s have surged to the forefront as a versatile nanostructured material in nanoelectronic applications. Polypeptides nanotubular structures with tunable properties offer a challenging alternative to CNT. Earlier experimental studies on L-Alanyl-L-Valine (AV) and L-Valyl-L-Alanine (VA) have demonstrated their potential as novel porous materials, which form channel-like structure (Soldatov et al., Angew. Chem. Int. Ed. 43, 6308 (2004)). In the study reported here, DFT calculations on two closely related cyclic dipeptides cyclo[Lalanyl-L-valine]3 and cyclo[L-valyl-L-alanine]3 and on their linear correlates, [L-alanyl-L-valine]3 and [L-valyl-L-alanine]3 have been performed. This paper presents the generalstructuraland electronic properties of cyclic and linear correlates of the nanotubular oligomeric dipeptides constructs, AV, and VA. We have compared the energy gaps of these cyclic rings and their linear correlates with that of other nanotubular constructs. The calculated HOMO–LUMO gap of these isolated ring structures is significantly larger than CNT’s. Further research is required to reduce the band gaps to be comparable to CNT’s and other inorganic tubular structures. Polypeptide design promises to be a major toolin engineering desirable band gap for the creation of novelnanostructured polypeptide nanotubes.