Structural and electronic properties of α-Te tubular nanostructures: a first-principles study

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We employed density functional theory to investigate the structural and electronic properties of α-Te tubular nanostructures. These α-Te tube-like structures, similar to that of carbon nanotubes, in armchair and zigzag types are semiconductors with moderate band gaps. The nanotubes in armchair configurations have an indirect-to-direct band gap transition as tube diameter is decreased to a specific critical tube size, while those in zigzag configurations are always semiconductors with direct gap independent of the tube diameter. The calculated projected density of states reveal that such an indirect-to-direct band gap transition found in armchair nanotube can be attributed to the contributions of the different p-orbitals near the VBM edges. These findings are not only helpful for better understanding the physical characteristics of α-Te nanotubes, but also will open up the possibility of its use in device applications.