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Structural properties and thermal stability of multi-walled black phosphorene nanotubes and its operation as temperature driven nanorotors[†]

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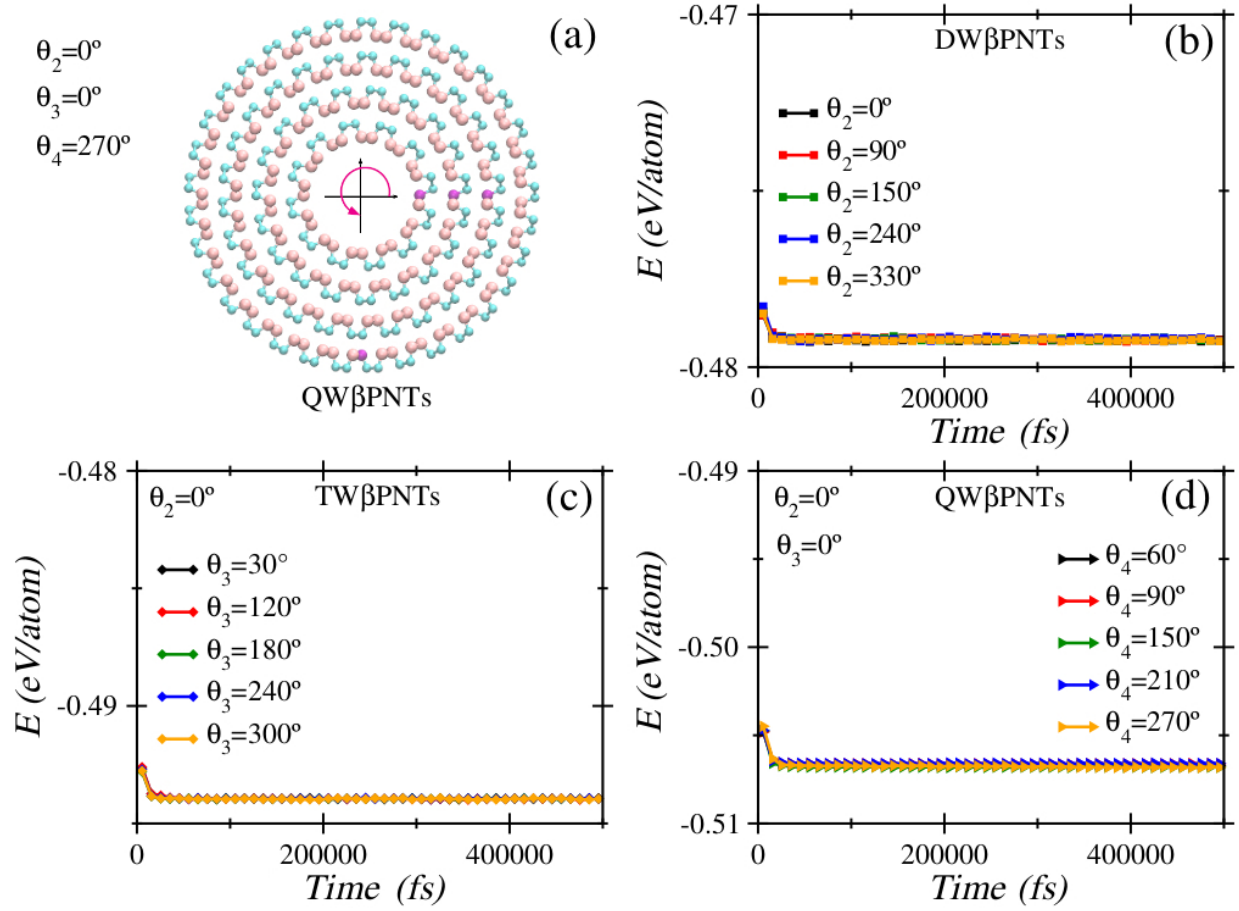


Fig. 1 (a) Rotation between the outer walls of a QWβPNT, with rotation angles of $\theta_2 = 0^\circ$, $\theta_3 = 0^\circ$, and $\theta_4 = 270^\circ$. Total energy/atom as function of MD time at room temperature for (b) DWβPNTs, (c) TWβPNTs, and (d) QWβPNT.

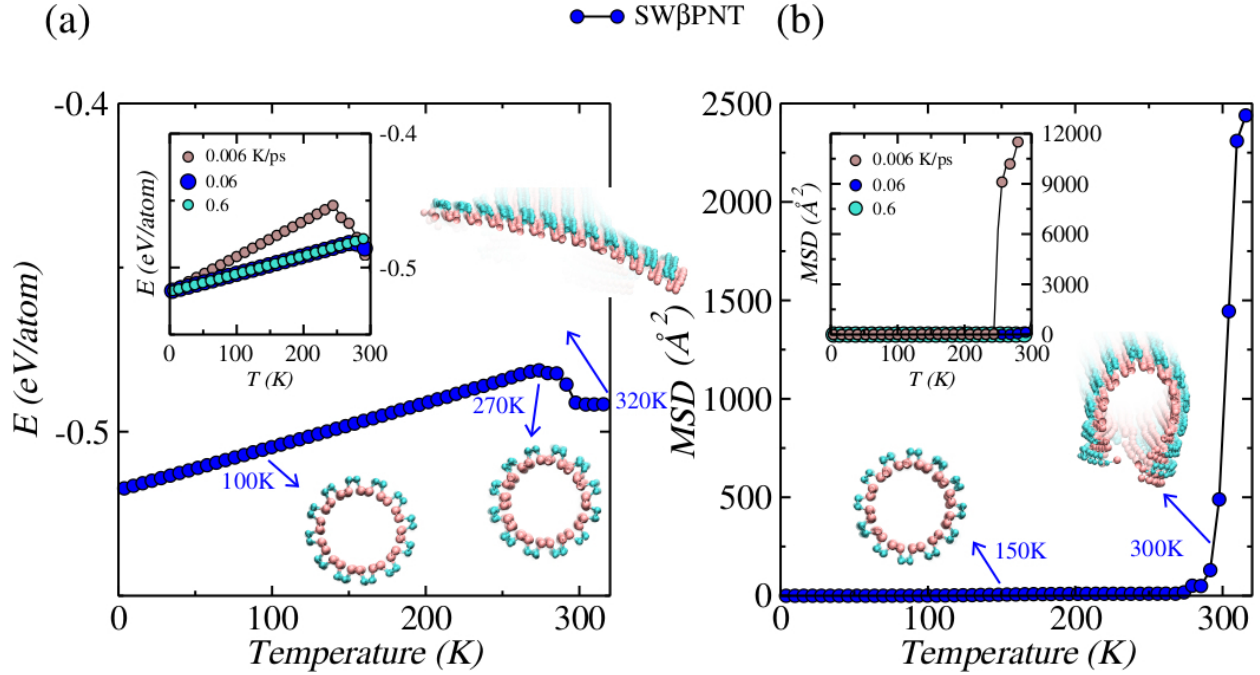


Fig. 2 (a) Total energy/atom as function of temperature, and (b) MSD as function of temperature during the heating process at a rate of 0.06 K/ps , for the SWβPNT. The inset boxes display $E(T)$ and MSD as a function of temperature for the SWβPNT with different heating rates (0.006 K/ps , 0.06 K/ps , and 0.6 K/ps). Selective snapshots (rate 0.06 K/ps) are shown at different temperatures.