Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary Information for

Adjustable 1D ferroelectricity and ferrielectricity in faceted GeSe nanotubes

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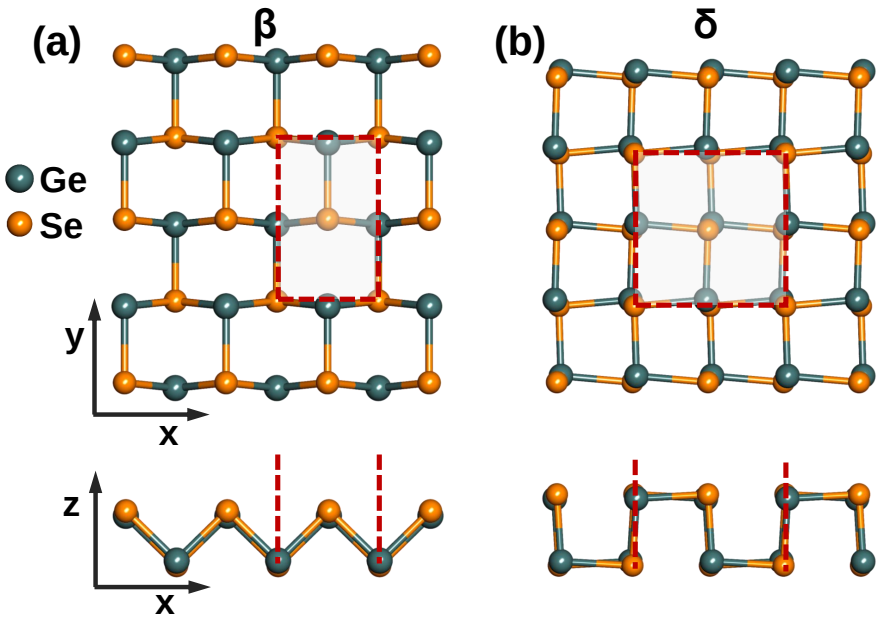

Figure S1: Equilibrium Structures of (a) β- and (b) δ-GeSe monolayers in both top and side views. The unit cells are indicated by red dashed lines.

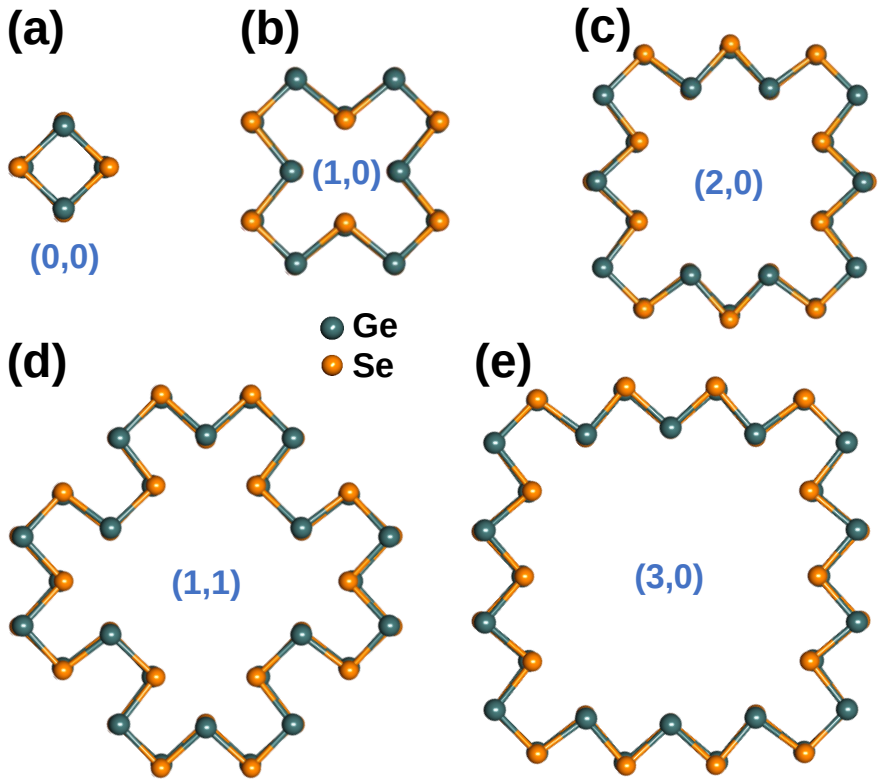

Figure S2: Equilibrium Structures of (a) (0,0)- (b) (1,0)-, (c) (2,0)-, (d) (1,1)-, and (e) (3,0)-GNTs in top view.

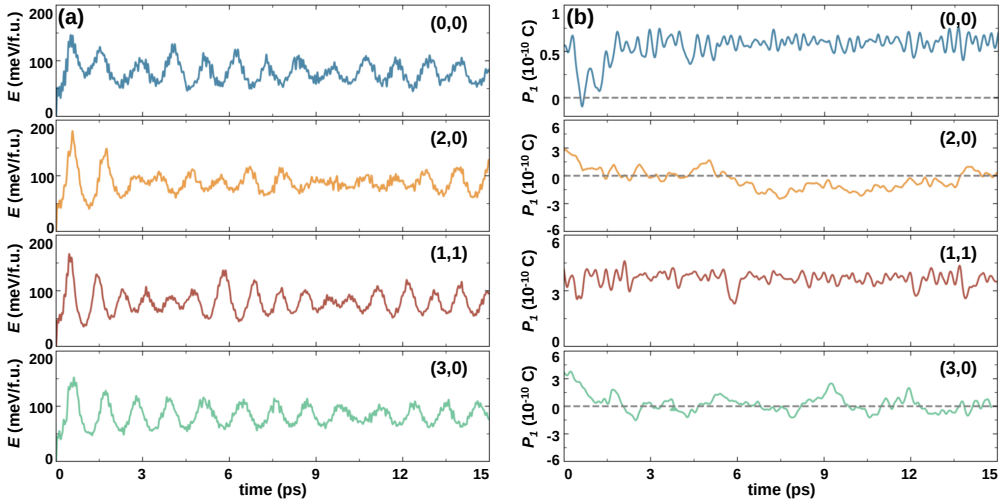

Figure S3: Fluctuations of the (a) total potential energy and (b) linear polarization (P_1) at 300 K for (0,0)-, (2,0)-, (1,1)-, and (3,0)-GNTs.

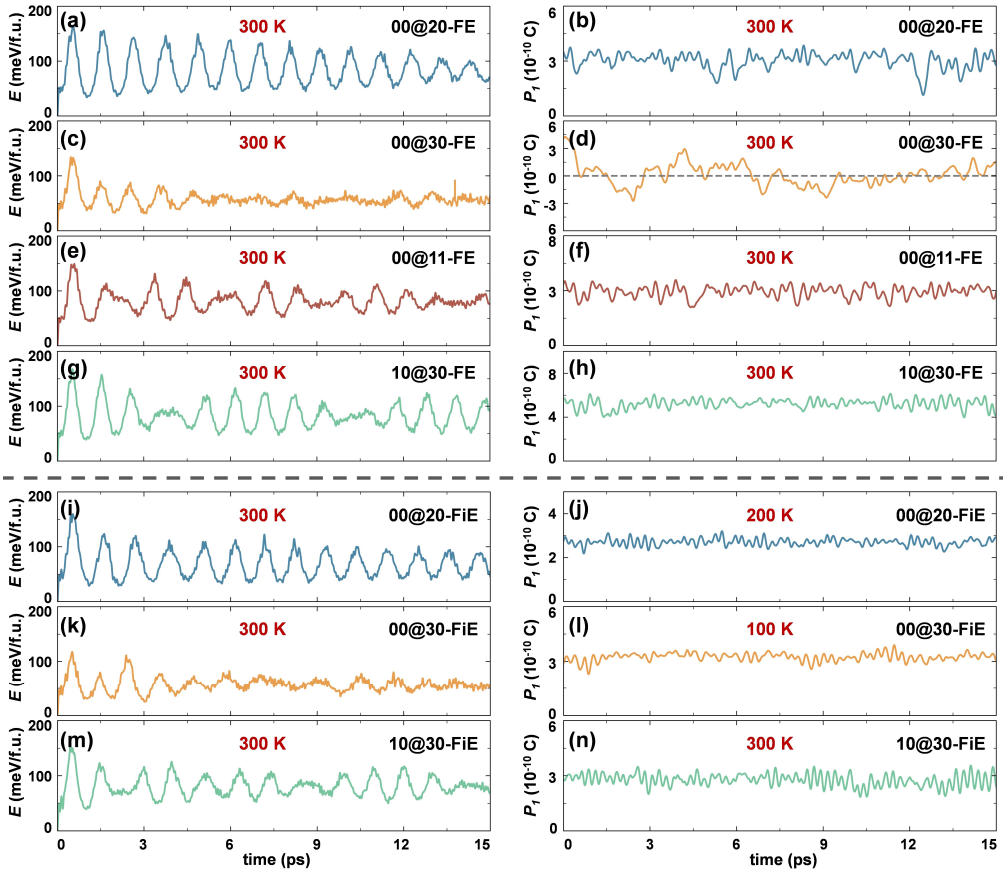

Figure S4: Fluctuations of the (a) total potential energy and (b) linear polarization (P_1) for the FE- and FiE-stacking (0,0)@(2,0)-, (0,0)@(3,0)-, (0,0)@(1,1)-, and (1,0)@(3,0)-GNTs at selected temperatures.

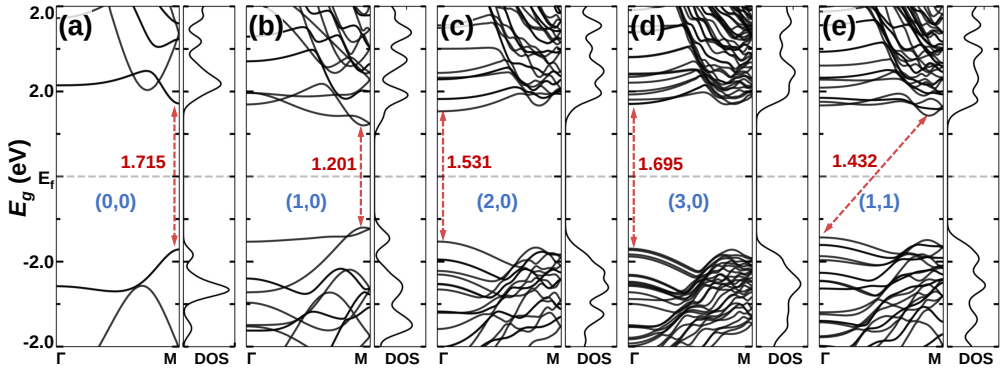

Figure S5: Electronic band structure and density of states (DOS) based on DFT-PBE for (a) (0,0)-, (b) (1,0)-, (c) (2,0)-, (d) (3,0)-, and (e) (1,1)-GNTs. The band gaps are indicated by dashed arrows and the corresponding values are given in the unit of eV.

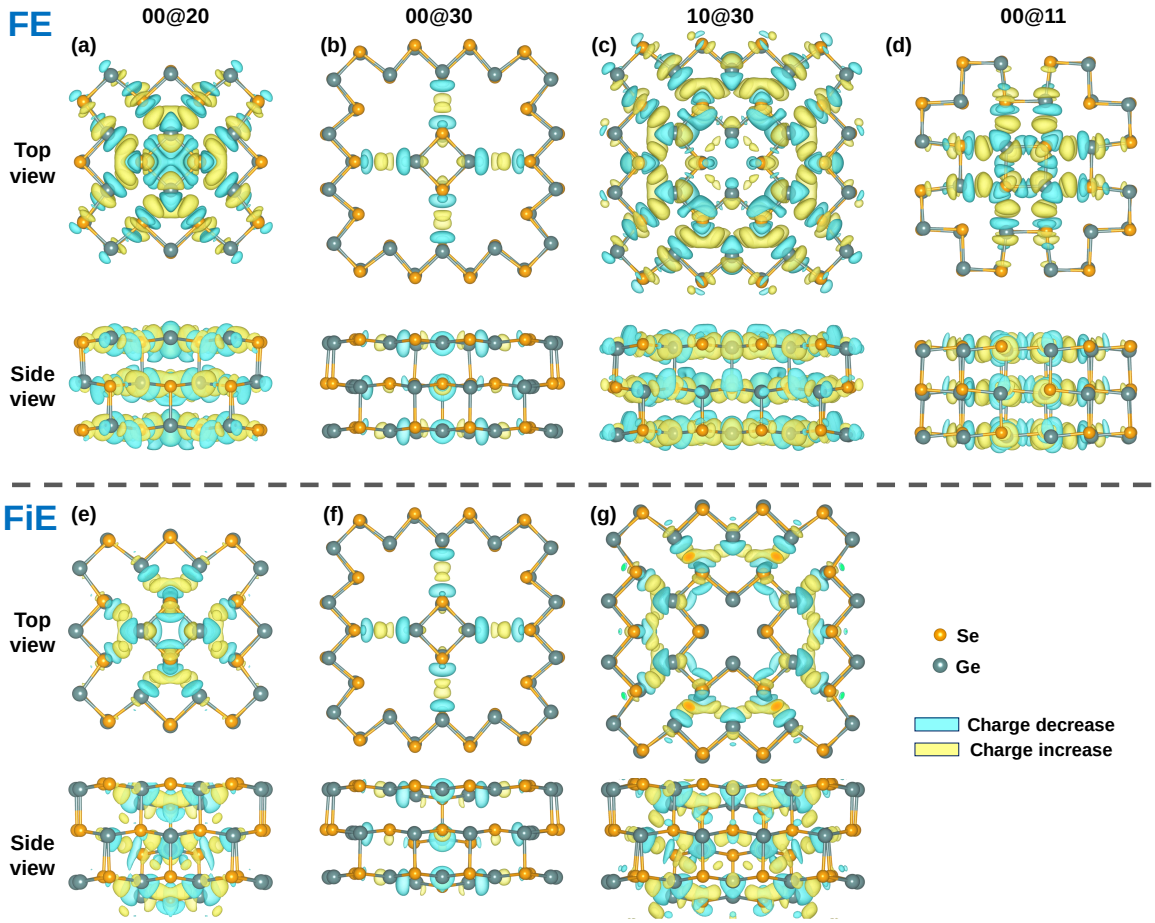

Figure S6: Differential charge density distribution for combining the DW FE-stacking (a) (0,0)@(2,0)-, (b) (0,0)@(3,0)-, (c) (1,0)@(3,0)-, (d) (0,0)@(1,1)-GNTs and FiE-stacking (e) (0,0)@(2,0)-, (f) (0,0)@(3,0)-, (g) (1,0)@(3,0)-GNTs. The yellow and blue isosurfaces represent the electron excess and deficit. The isosurface value for (0,0)@(3,0)-GNT is 0.0002 e/Bohr^3 and that for the others is 0.001 e/Bohr^3.