Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Dimension Effect on Ferroelectricity: A First-principles Study in GeS Nanoribbons

Haishan Su[1],Ting Hu[1,*], Erjun Kan[1]

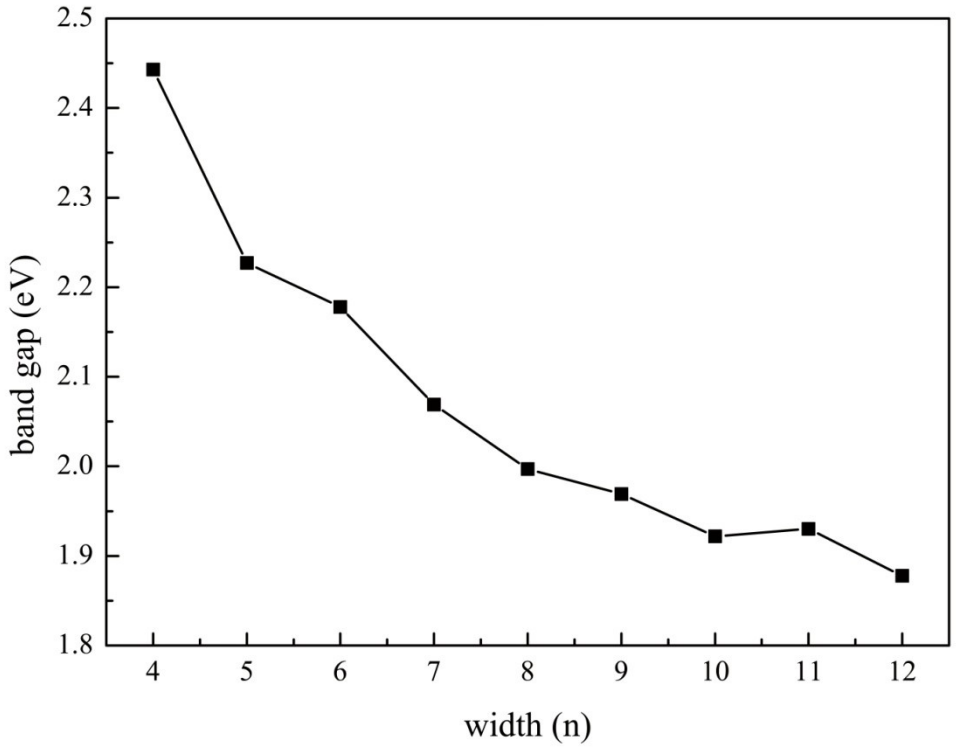

Figure S1 The band gap H-terminated A-GeSNRs varies with ribbon width.

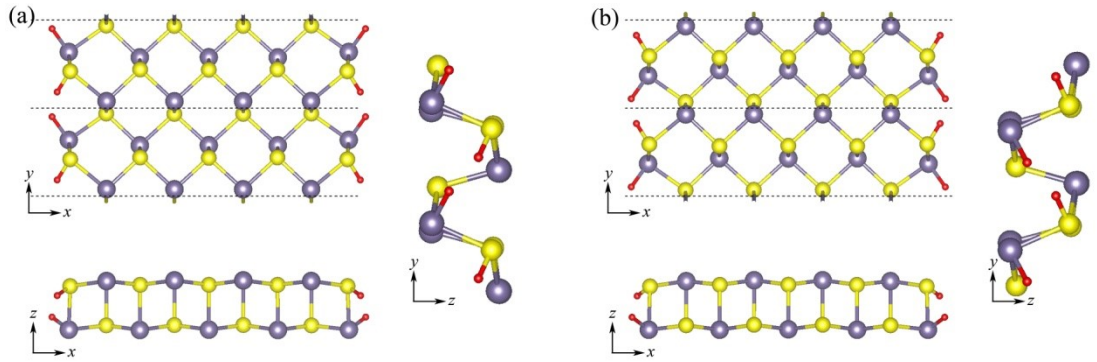

Figure S2 The geometric structures of 9-H-A-GeSNR with opposite polarization directions.

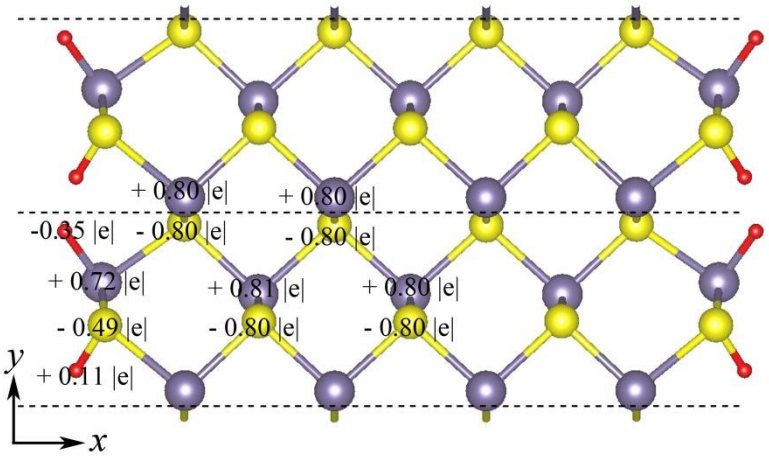

Figure S3 The charge distribution of 9-H-A-GeSNR.

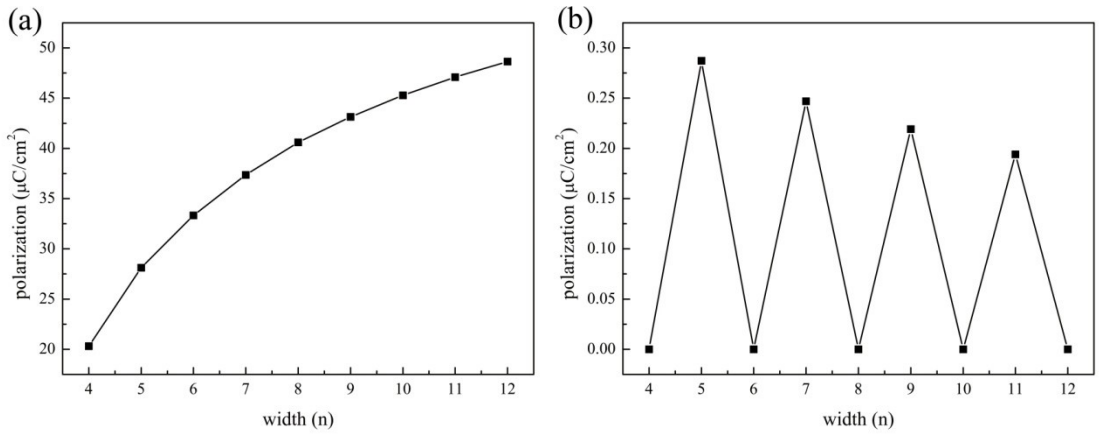

Figure S4 Ferroelectric polarizations of H-A-GeSeNR along (a) ribbon direction and (b) out-of-plane direction as a function of ribbon width.

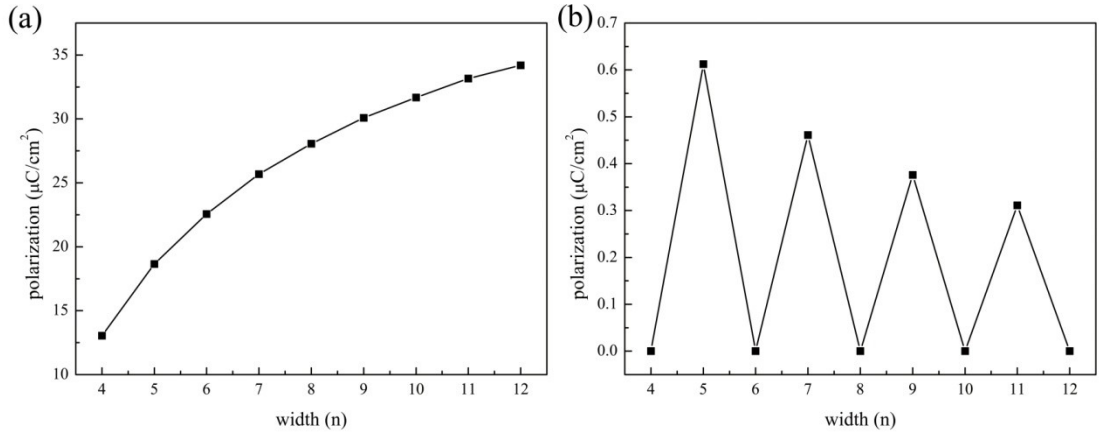

Figure S5 Ferroelectric polarizations of H-A-SnSNR along (a) ribbon direction and (b) out-of-plane direction as a function of ribbon width.

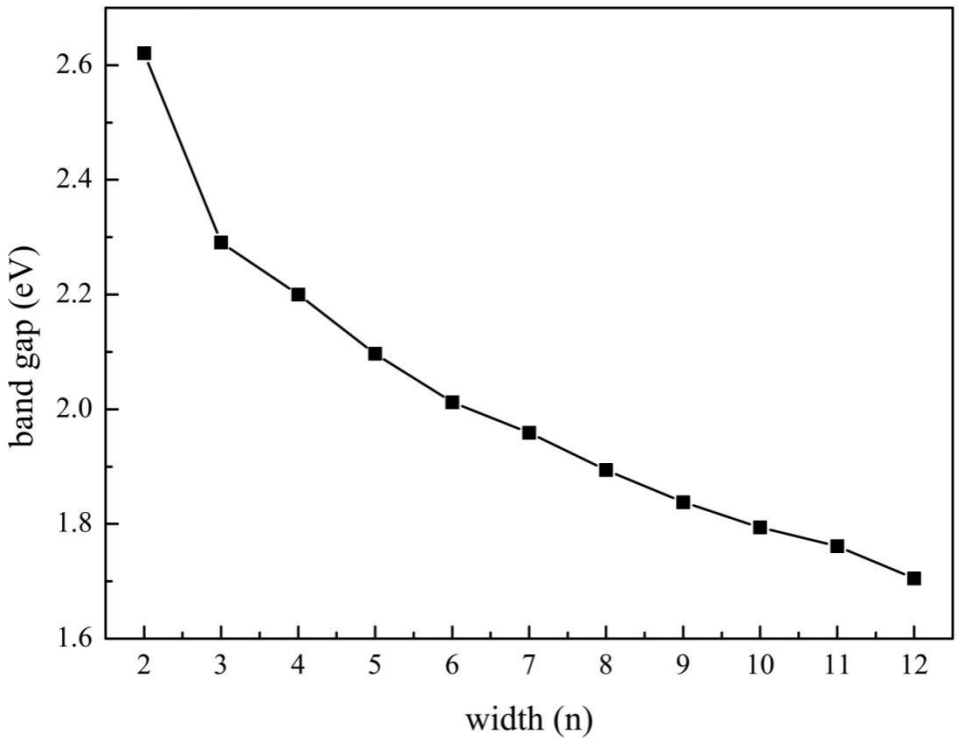

Figure S6 The band gap H-terminated Z-GeSNRs varies with ribbon width.

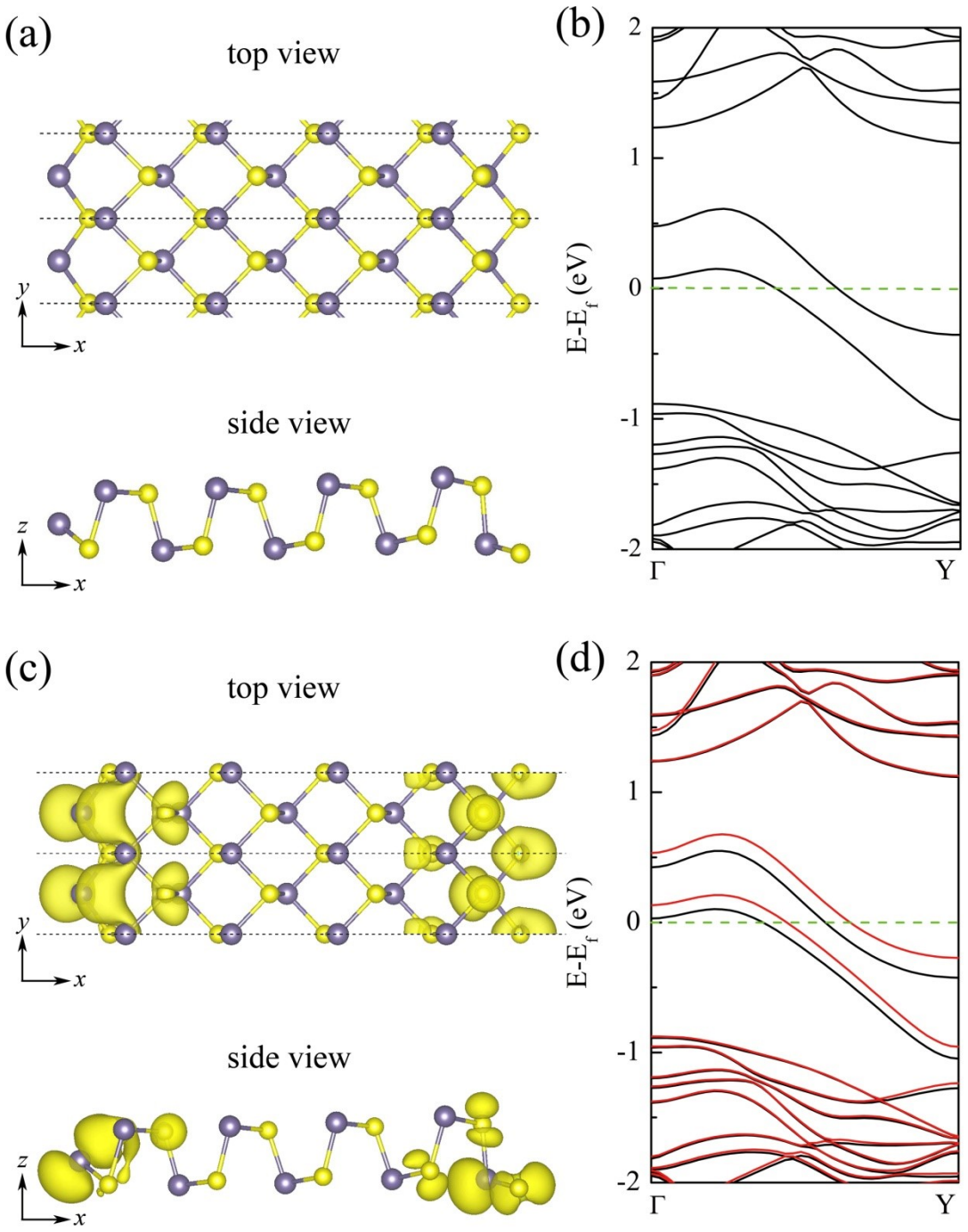

Figure S7 (a) Top and side views for the optimized geometric structures of 9-Z-GeSNR. The Ge, S and H atoms are denoted by purple, yellow and red dots, respectively. (b) The band structure of 9-Z-GeSNR. (c) The spin-polarized charge densities of the 9-Z-GeSNR in the FM state. (d) The spin polarized band structure of 9-Z-GeSNR in the FM state.