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

A Detailed Study on the Electronic and Optical Properties of Germanium Nanotubes

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Supplementary Materials

Table S1: The lowest conduction band energy E_{LCB}, the highest valence band energy E_{HVB}, and the energy gap E_g, where $E_g = E_{LCB} - E_{HVB}$.

aGeNTs	E_{LCB} (eV)	E_{HVB} (eV)	E_g (eV)
Ge(2,2)	0.360	-0.210	0.57
Ge(3,3)	0.040	-0.040	0.08
Ge(4,4)	0.294	-0.205	0.50
Ge(5,5)	0.290	-0.210	0.50
Ge(6,6)	0.205	-0.205	0.41
Ge(7,7)	0.170	-0.170	0.34
Ge(8,8)	0.150	-0.150	0.30
Ge(9,9)	0.130	-0.130	0.26
Ge(10,10)	0.125	-0.115	0.24
Ge(11,11)	0.100	-0.100	0.20
Ge(12,12)	0.098	-0.092	0.19
Ge(13,13)	0.090	-0.090	0.18
Ge(15,15)	0.075	-0.075	0.15

zGeNTs	E_{LCB} (eV)	E_{HVB} (eV)	E_g (eV)
Ge(4,0)	-	-	0
Ge(5,0)	-	-	0
Ge(6,0)	-	-	0
Ge(7,0)	-	-	0
Ge(8,0)	0.090	-0.090	0.18
Ge(9,0)	0.130	-0.130	0.26
Ge(10,0)	0.200	-0.200	0.40
Ge(11,0)	0.200	-0.200	0.40
Ge(13,0)	0.230	-0.210	0.44
Ge(15,0)	0.160	-0.120	0.28
Ge(21,0)	0.04	-0.140	0.18
Ge(27,0)	0.04	-0.100	0.14

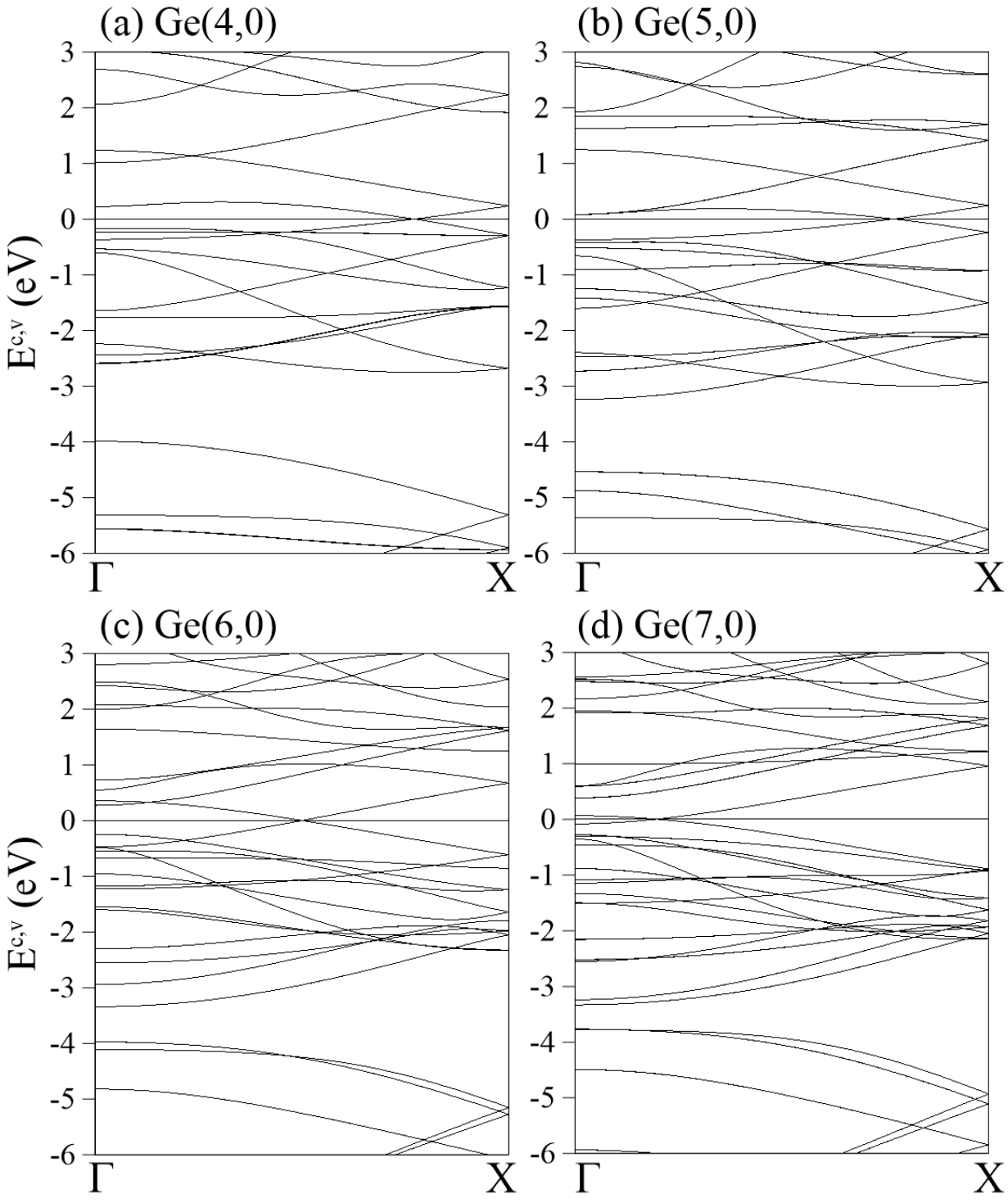

Figure S1: Band structures of metallic zGeNTs with different chiral vectors: (a) (4,0), (b) (5,0), (c) (6,0), and (d) (7,0).

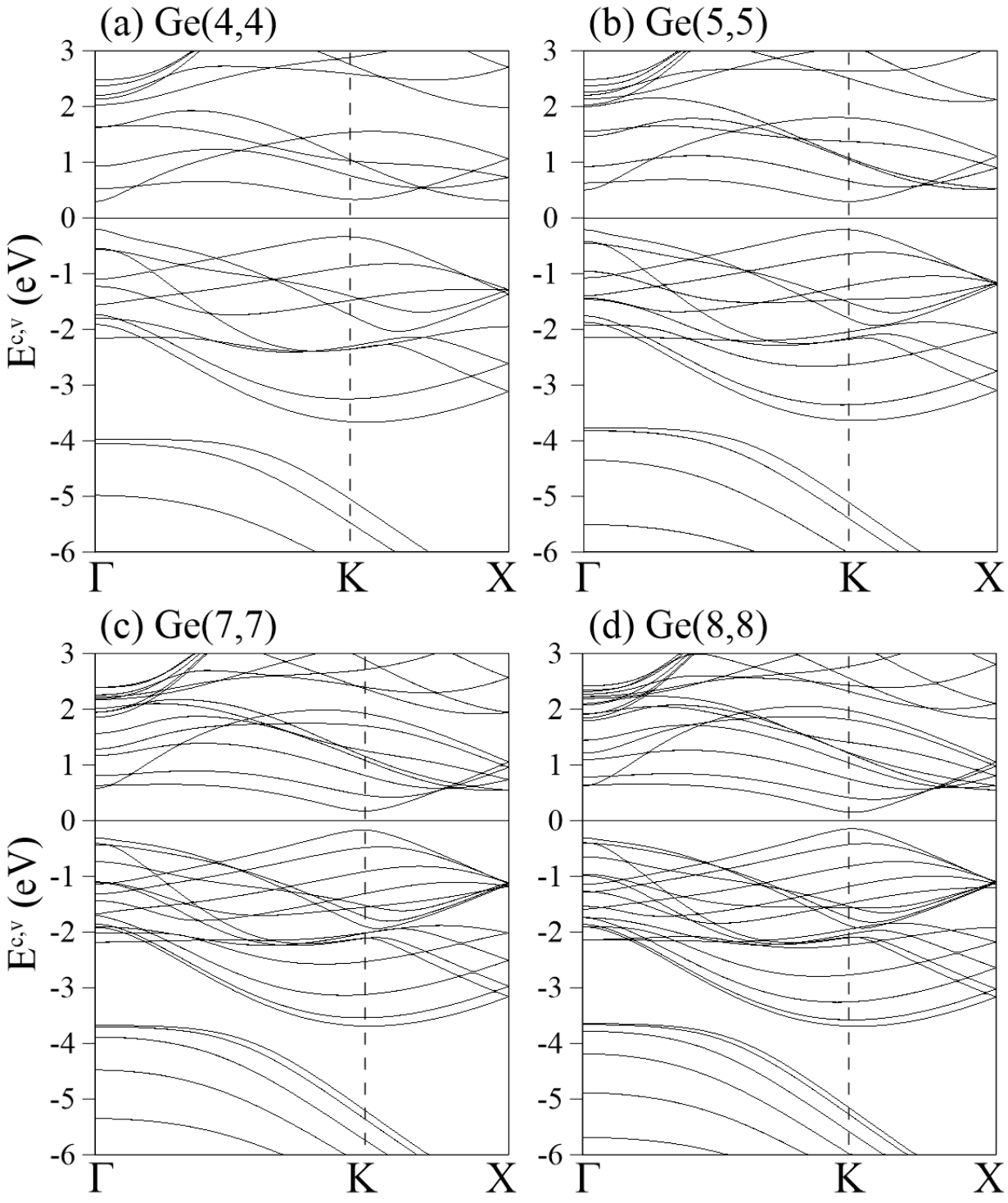

Figure S2: Band structures of aGeNTs with different chiral vectors: (a) (4,4), (b) (5,5), (c) (7,7), and (d) (8,8).

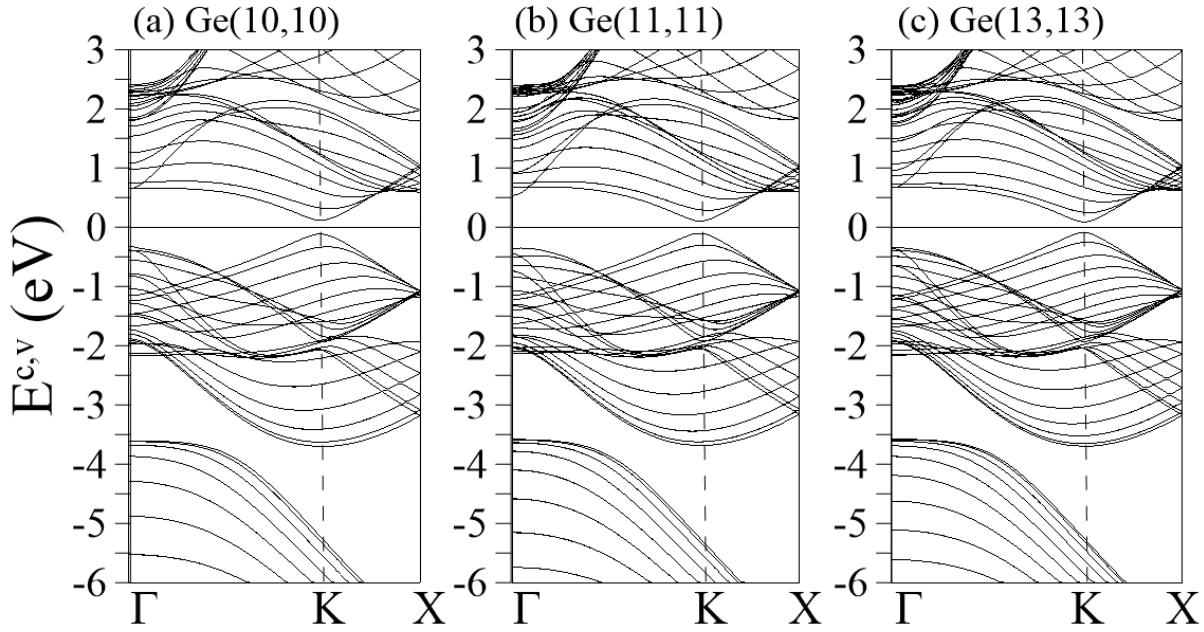

Figure S3: Band structures of aGeNTs with different chiral vectors: (a) (10,10), (b) (11,11), and (c) (13,13).

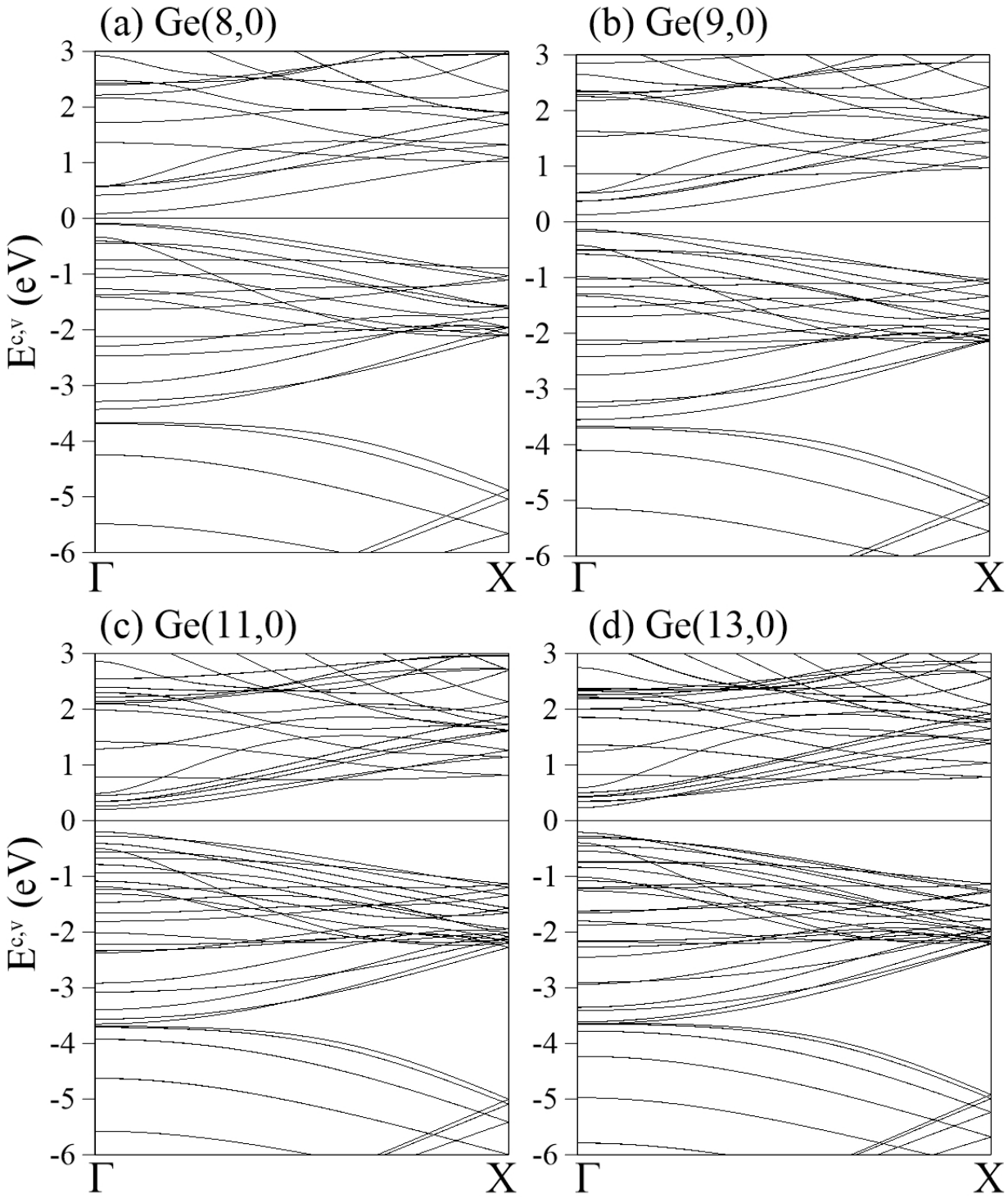

Figure S4: Band structures of zGeNTs with different chiral vectors: (a) (8,0), (b) (9,0), (c) (11,0), and (d) (13,0).