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**Electronic Supplementary Information**

# First-Principles Studies of the Thermoelectric Properties of [110]-Ge/Si Core/Shell Nanowires with Different Surface Structures

*Jin-Ni Shen,* [†, ‡, &], *Li-Ming Wu,* [*, †] *Yong-Fan Zhang*[§]

[†] *State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, People's Republic of China;*

[‡] *Key Laboratory of Design and Assembly of Functional nanostructures, Chinese Academy of Sciences, Fuzhou, Fujian 350002, People's Republic of China.*

[&] *University of Chinese Academy of Sciences, Beijing 100039, People's Republic of China*

[§] *Department of Chemistry, Fuzhou University, Fujian 350108, People's Republic of China.*

To whom correspondence should be addressed. E-mail: liming_wu@fjirsm.ac.cn. Tel: (011)86-591-83705401.

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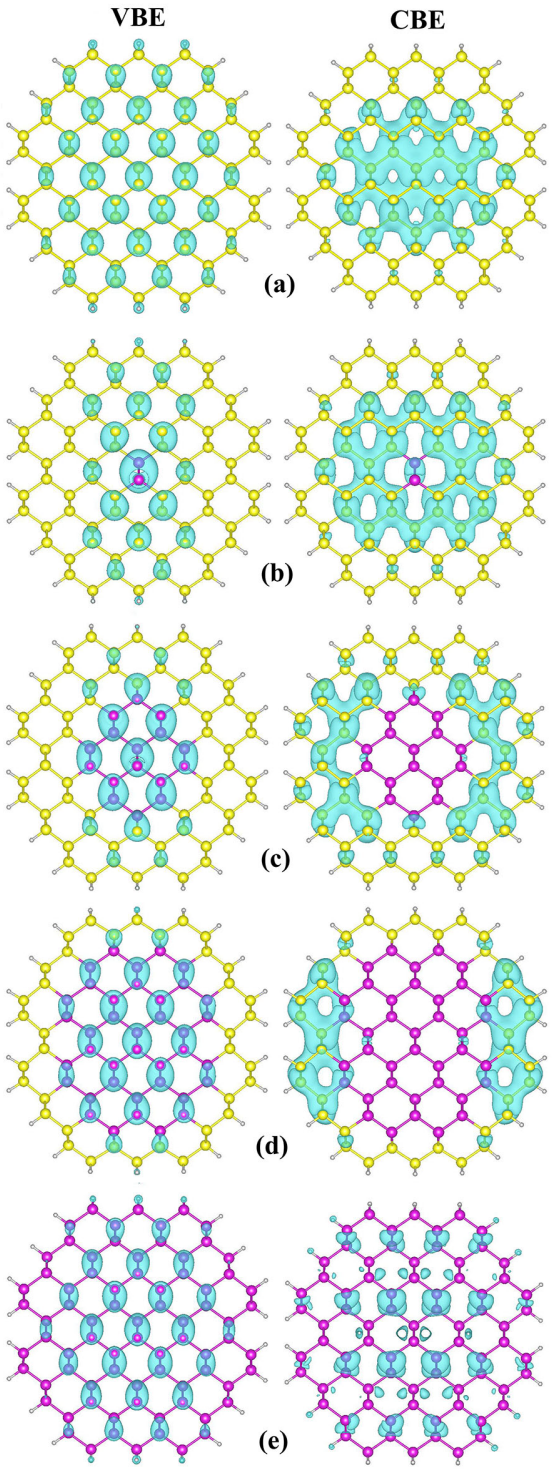


**Fig. S1.** Isosurface charge densities of VBE (left column) and CBE (right column) for [110]-Ge/Si core/shell NWs with **S** surface structure. (a) **S**-SiNW, (b) **S**-Ge/Si_#1, (c) **S**-Ge/Si_#2, (d) **S**-Ge/Si_#3, (e) **S**-GeNW. The yellow, magenta, and gray spheres represent Si, Ge, and H atoms, respectively. The density of isosurfaces (displayed by blue pixels) is $5\times10^{-4}$ e/Å$^3$.

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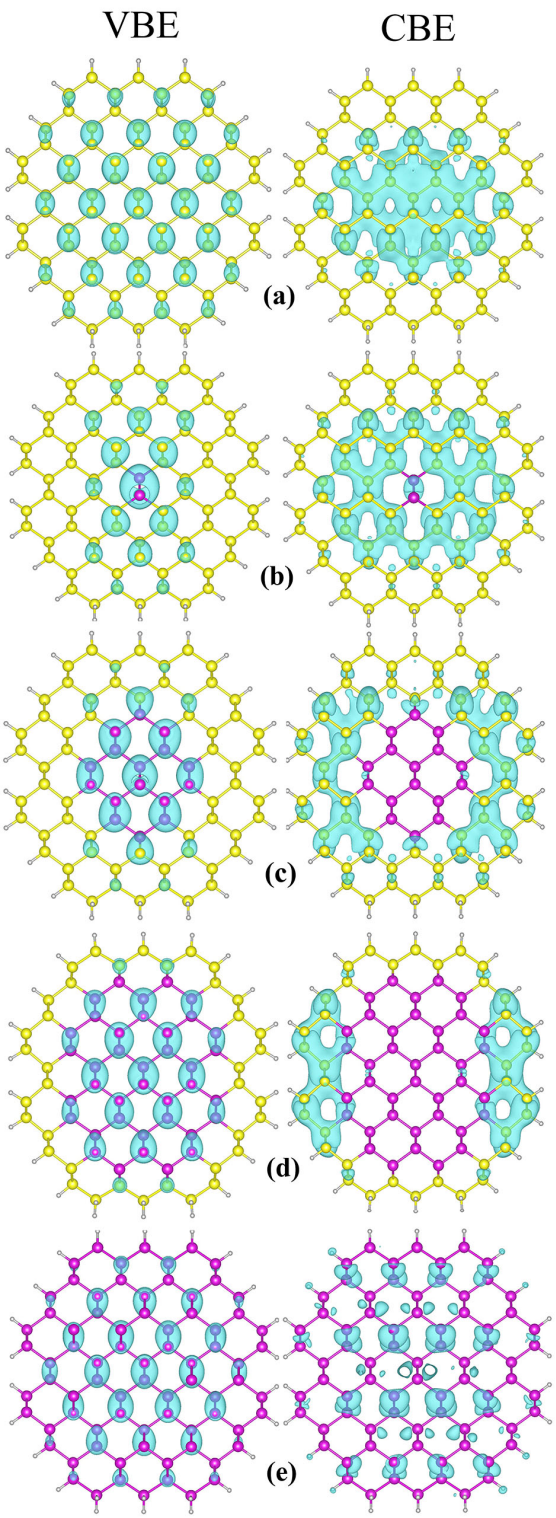


**Fig. S2.** Isosurface charge densities of VBE (left column) and CBE (right column) for [110]-Ge/Si core/shell NWs with **C** surface structure. (a) **C**-SiNW, (b) **C**-Ge/Si_#1, (c) **C**-Ge/Si_#2, (d) **C**-Ge/Si_#3, (e) **C**-GeNW. The yellow, magenta, and gray spheres represent Si, Ge, and H atoms, respectively. The density of isosurfaces (displayed by blue pixels) is $5\times10^{-4}$ e/Å$^3$.

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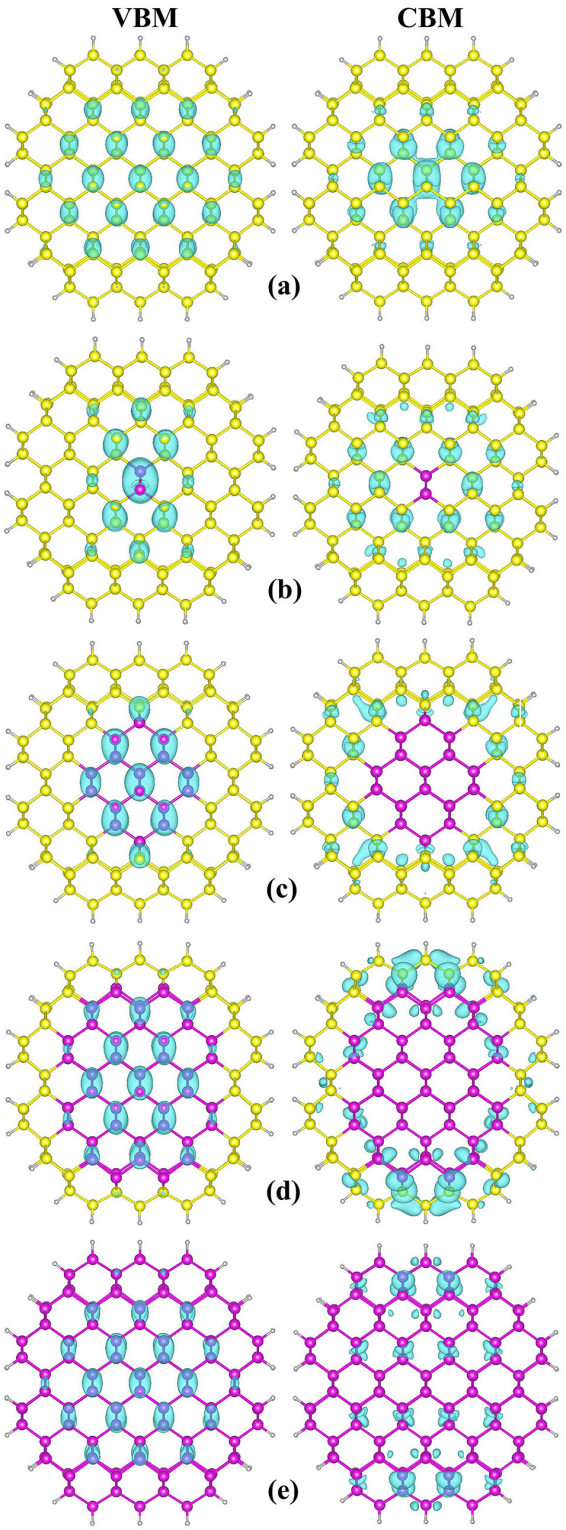


**Fig. S3.** Isosurface charge densities of VBE (left column) and CBE (right column) for [110]-Ge/Si core/shell NWs with **R** surface structure. (a) **R**-SiNW, (b) **R**-Ge/Si_#1, (c) **R**-Ge/Si_#2, (d) **R**-Ge/Si_#3, (e) **R**-GeNW. The yellow, magenta, and gray spheres represent Si, Ge, and H atoms, respectively. The density of isosurfaces (displayed by blue pixels) is $5\times10^{-4}$ e/Å$^3$.

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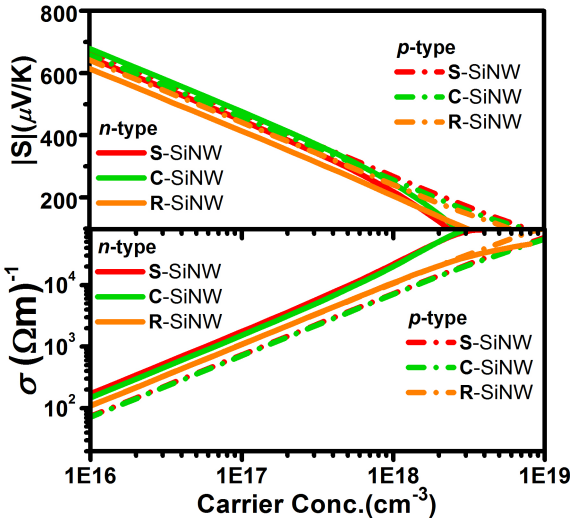


**Fig. S4.** Calculated $S$ (upper panel), and $\sigma$ (lower panel) as a function of carrier concentration for SiNW with three different surface structures: **S** (red), **C** (green), and **R** (orange). The solid and dash lines denote *n*-type and *p*-type, respectively.

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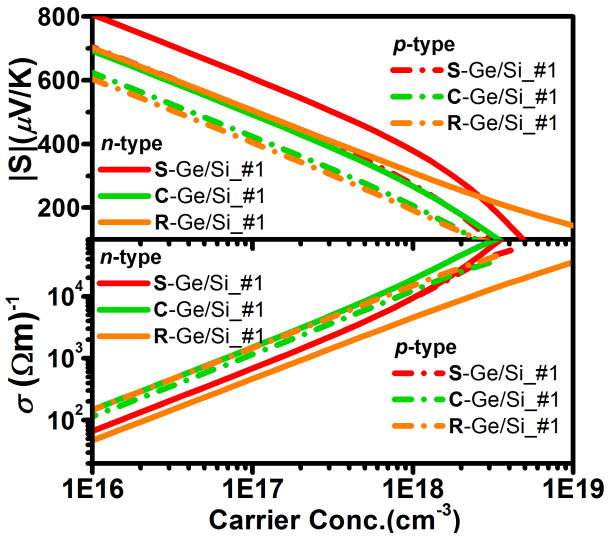


**Fig. S5.** Calculated $S$ (upper panel), and $\sigma$ (lower panel) as a function of carrier concentration for [110]-Ge/Si_#1 with three different surface structures: **S** (red), **C** (green), and **R** (orange). The solid and dash lines denote *n*-type and *p*-type, respectively.

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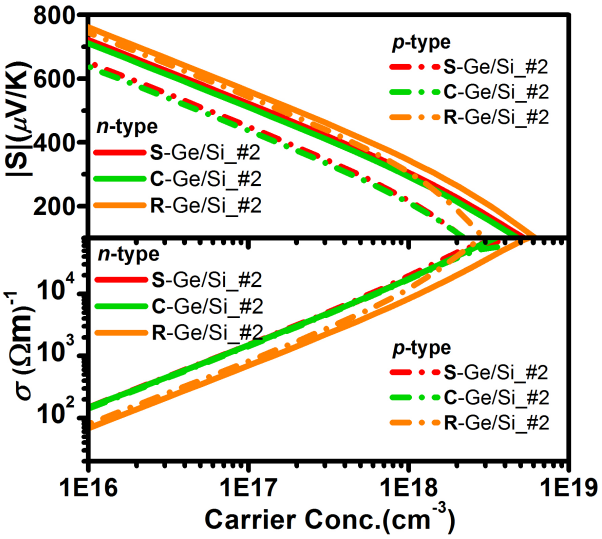


**Fig. S6.** Calculated $S$ (upper panel), and $\sigma$ (lower panel) as a function of carrier concentration for [110]-Ge/Si_#2 with three different surface structures: **S** (red), **C** (green), and **R** (orange). The solid and dash lines denote *n*-type and *p*-type, respectively.

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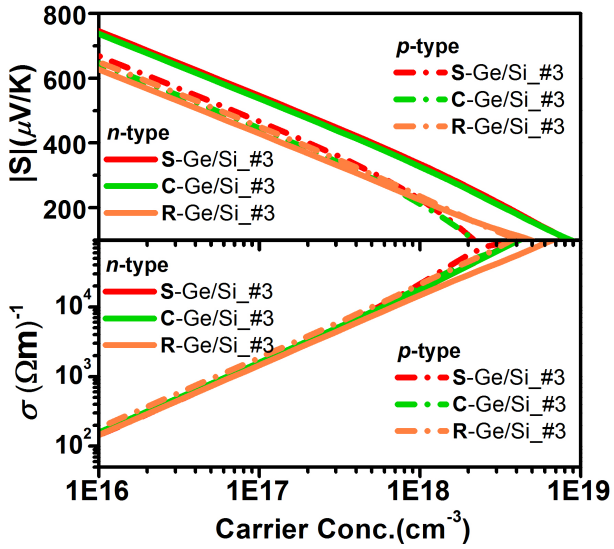


**Fig. S7.** Calculated $S$ (upper panel), and $\sigma$ (lower panel) as a function of carrier concentration for [110]-Ge/Si_#3 with three different surface structures: **S** (red), **C** (green), and **R** (orange). The solid and dash lines denote *n*-type and *p*-type, respectively.

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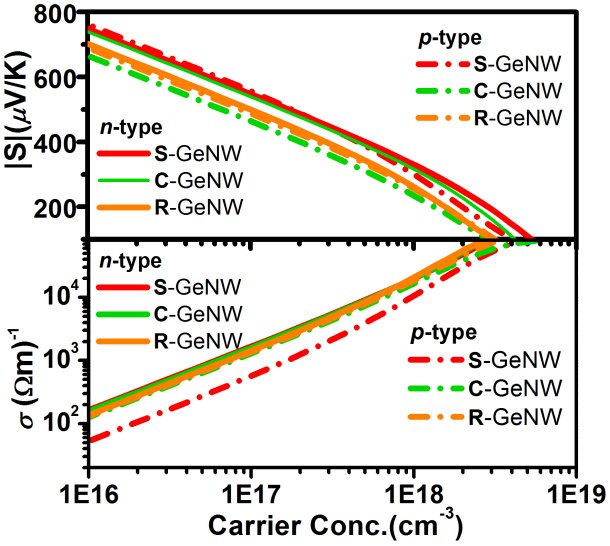


**Fig. S8.** Calculated $S$ (upper panel), and $\sigma$ (lower panel) as a function of carrier concentration for [110]-GeNW with three different surface structures: **S** (red), **C** (green), and **R** (orange). The solid and dash lines denote *n*-type and *p*-type, respectively.