

Supplementary File 1

Band structures and total density of states (TDOS) diagrams for the double ($x=16.6\%$) Al/Ga-doped (6,0) SWSiCNT system at Si/C sites.

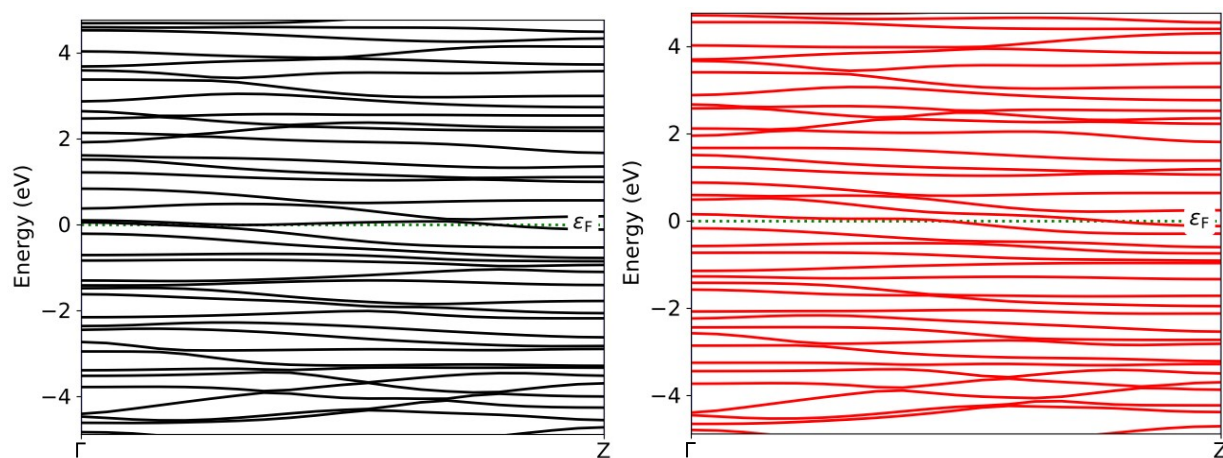


Fig. 1. The calculated spin-up (black) and spin-down (red) band structures for $\text{Si}_{10}\text{Al}_2\text{C}_{12}$ NTs.

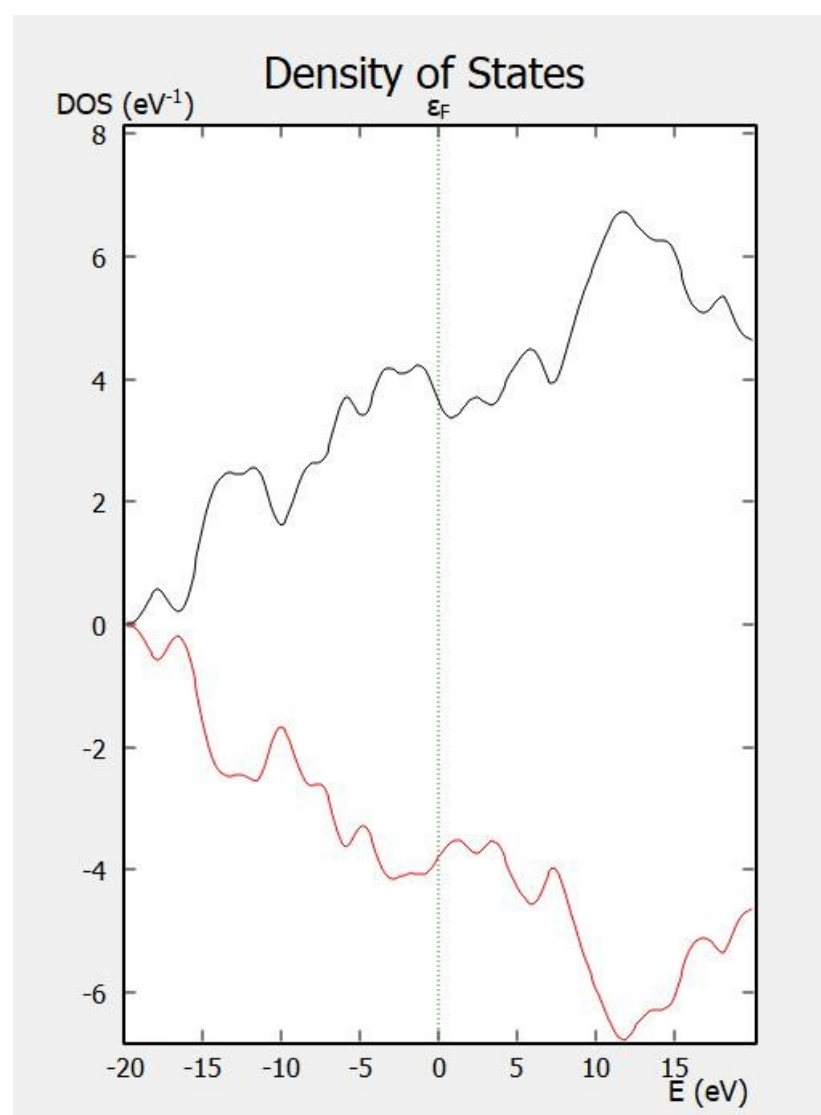


Fig. 2. The calculated TDOS diagram for $\text{Si}_{10}\text{Al}_2\text{C}_{12}$ NTs.

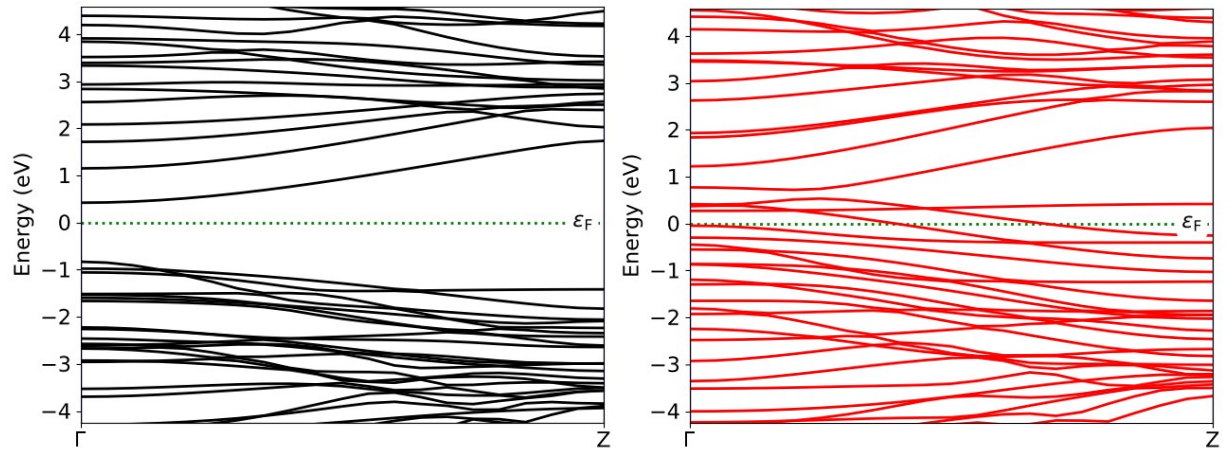


Fig. 3. The calculated spin-up (black) and spin-down (red) band structures for $\text{Si}_{10}\text{Ga}_2\text{C}_{12}$ NTs.

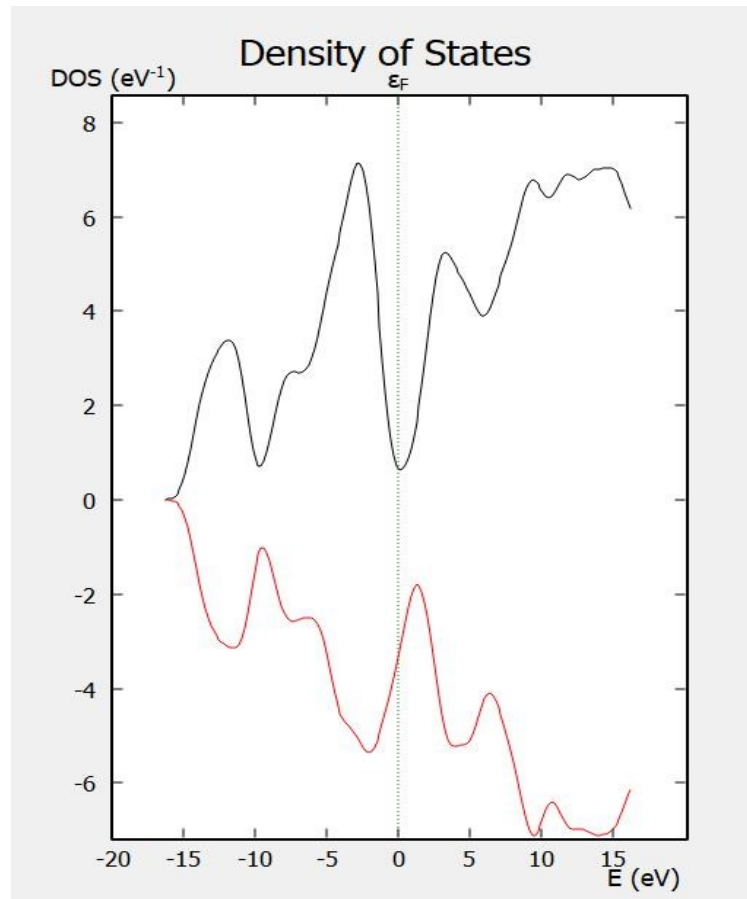


Fig. 4. The calculated TDOS diagram for $\text{Si}_{10}\text{Ga}_2\text{C}_{12}$ NTs.

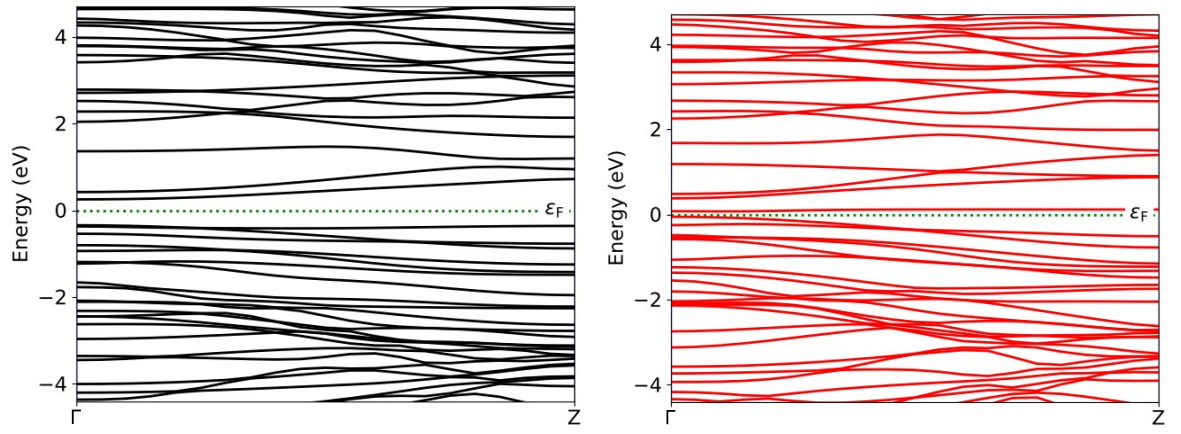


Fig. 5. The calculated spin-up (black) and spin-down (red) band structures for $\text{Si}_{12}\text{C}_{10}\text{Al}_2$ NTs.

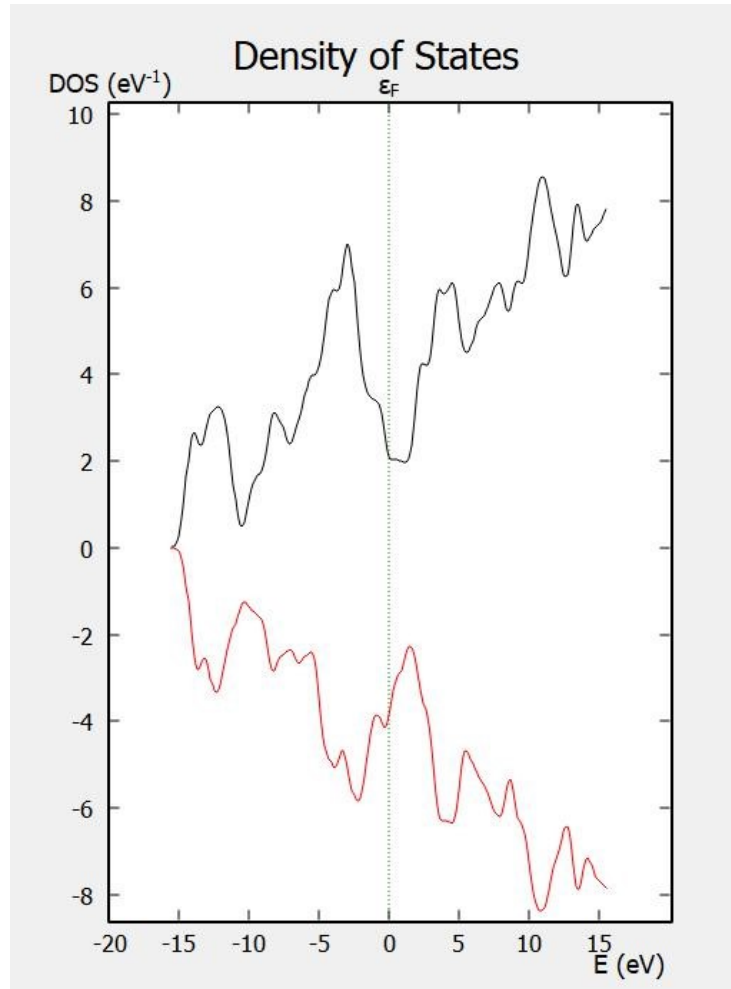


Fig. 6. The calculated TDOS diagram for $\text{Si}_{12}\text{C}_{10}\text{Al}_2$ NTs.

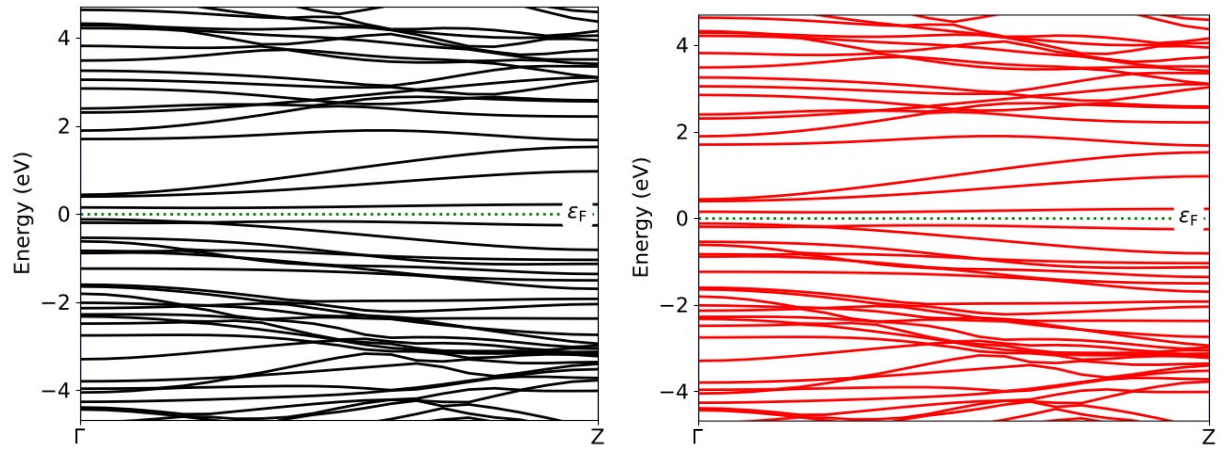


Fig. 7. The calculated spin-up (black) and spin-down (red) band structures for $\text{Si}_{12}\text{C}_{10}\text{Ga}_2$ NTs.

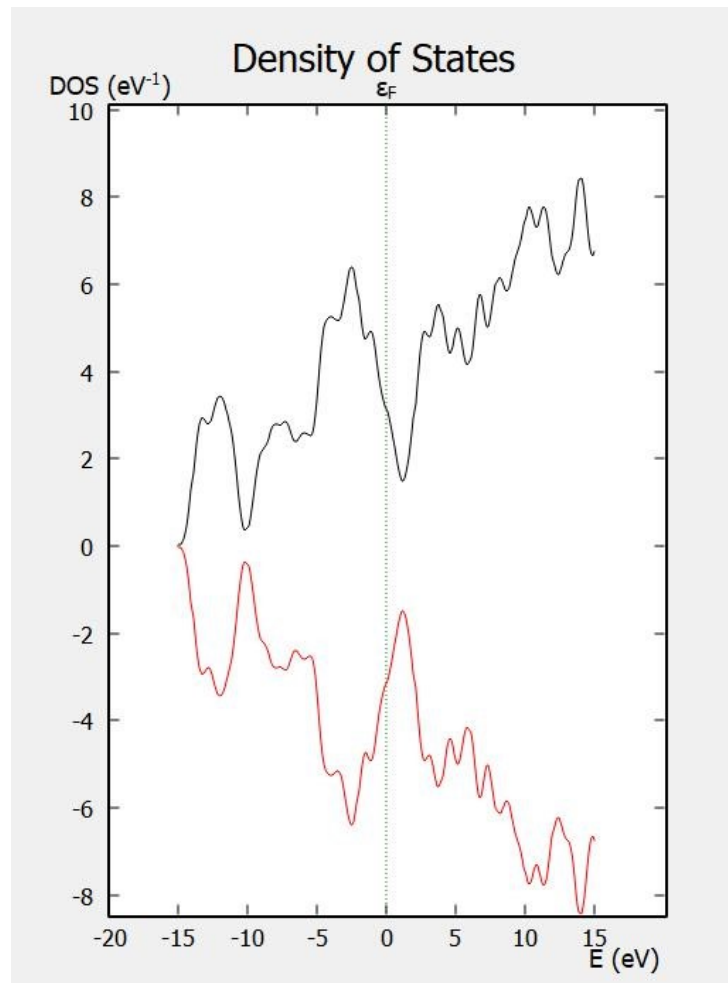


Fig. 8. The calculated TDOS diagram for $\text{Si}_{12}\text{C}_{10}\text{Ga}_2$ NTs.