Supplementary Information (SI) for Physical Chemistry Chemical Physics. This journal is © the Owner Societies 2025

Supplementary File 1

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

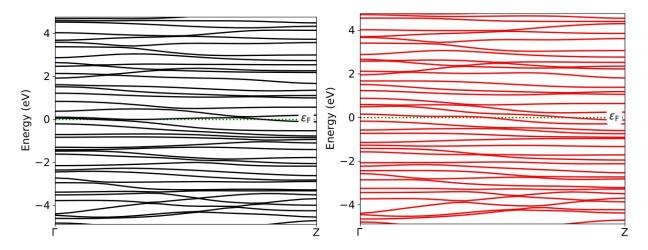


Fig. 1. The calculated spin-up (black) and spin-down (red) band structures for Si₁₀Al₂C₁₂ NTs.

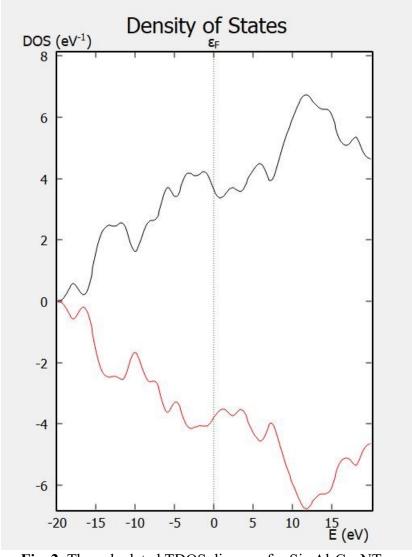
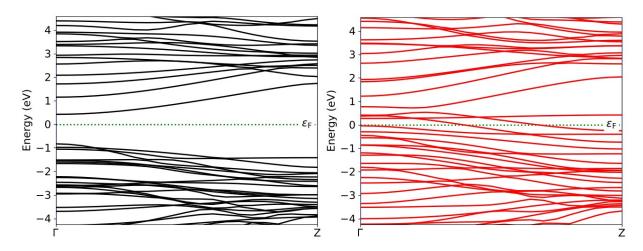


Fig. 2. The calculated TDOS diagram for $Si_{10}Al_2C_{12}$ NTs.



 $\textbf{Fig. 3.} \ \ \text{The calculated spin-up (black) and spin-down (red) band structures for } Si_{10}Ga_2C_{12}\ NTs.$

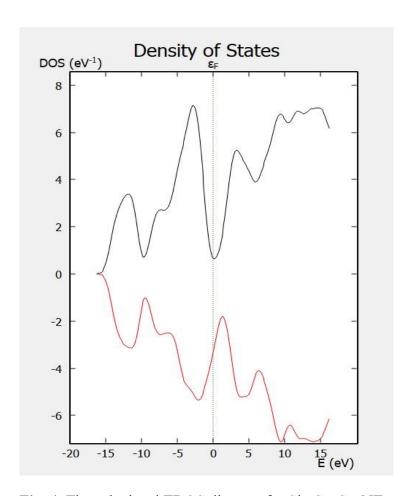
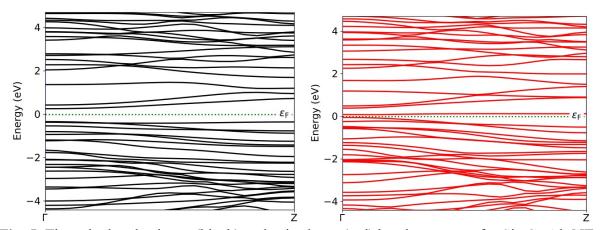


Fig. 4. The calculated TDOS diagram for $\rm Si_{10}Ga_2C_{12}$ NTs.



 $\textbf{Fig. 5.} \ \ \text{The calculated spin-up (black) and spin-down (red) band structures for } Si_{12}C_{10}Al_2\ NTs.$

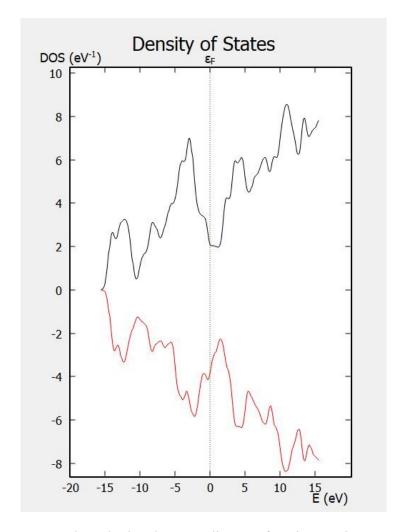


Fig. 6. The calculated TDOS diagram for $Si_{12}C_{10}Al_2$ NTs.

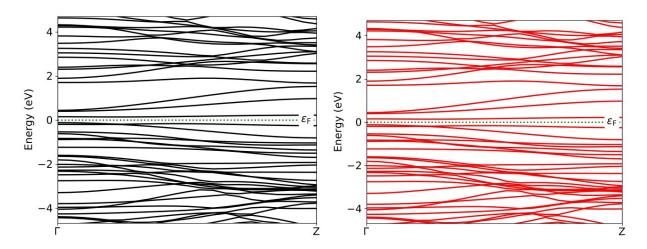


Fig. 7. The calculated spin-up (black) and spin-down (red) band structures for $Si_{12}C_{10}Ga_2$ NTs.

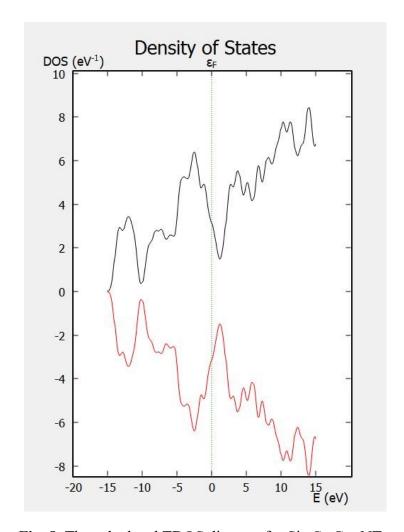


Fig. 8. The calculated TDOS diagram for $\rm Si_{12}C_{10}Ga_2$ NTs.