Tuning from half-metallic to semiconducting behavior in SiC nanoribbons

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The fully relaxed bare-edged -$[SiC]_7$-(2) ribbon for the second of the two energetically degenerate magnetic ground states, noted as (↑↑ - ↓↓), does not exhibit noticeable geometrical differences with respect to its counterpart noted as (↑↑ - ↑↑). Si atoms, denoted by Si-1 and Si-2 in Figure S1, are non-equivalent atoms as to what they show a relative lateral displacement of 0.2 Å at the zigzag edge. The spin density distribution of the ground state of -$[SiC]_7$-(2) noted with (↑↑ - ↓↓) exhibits the same ferromagnetic alignment of spins along the edges, but pointing out in opposite directions across the ribbon width. As a result, the system becomes fully-metallic as shown in the spin-resolved band diagram in Figure S1-c), with a total magnetic moment of -1.25 μ_B. For this ribbon, the projected density of states (PDoS) of Si-1 and Si-2 edge atoms are plotted in Figure S1 d) and e), respectively, and reveal that the metallic character of the ribbon comes from the p_x-orbitals of C and the p_y-orbitals of Si-2 atoms at the ribbon edge.

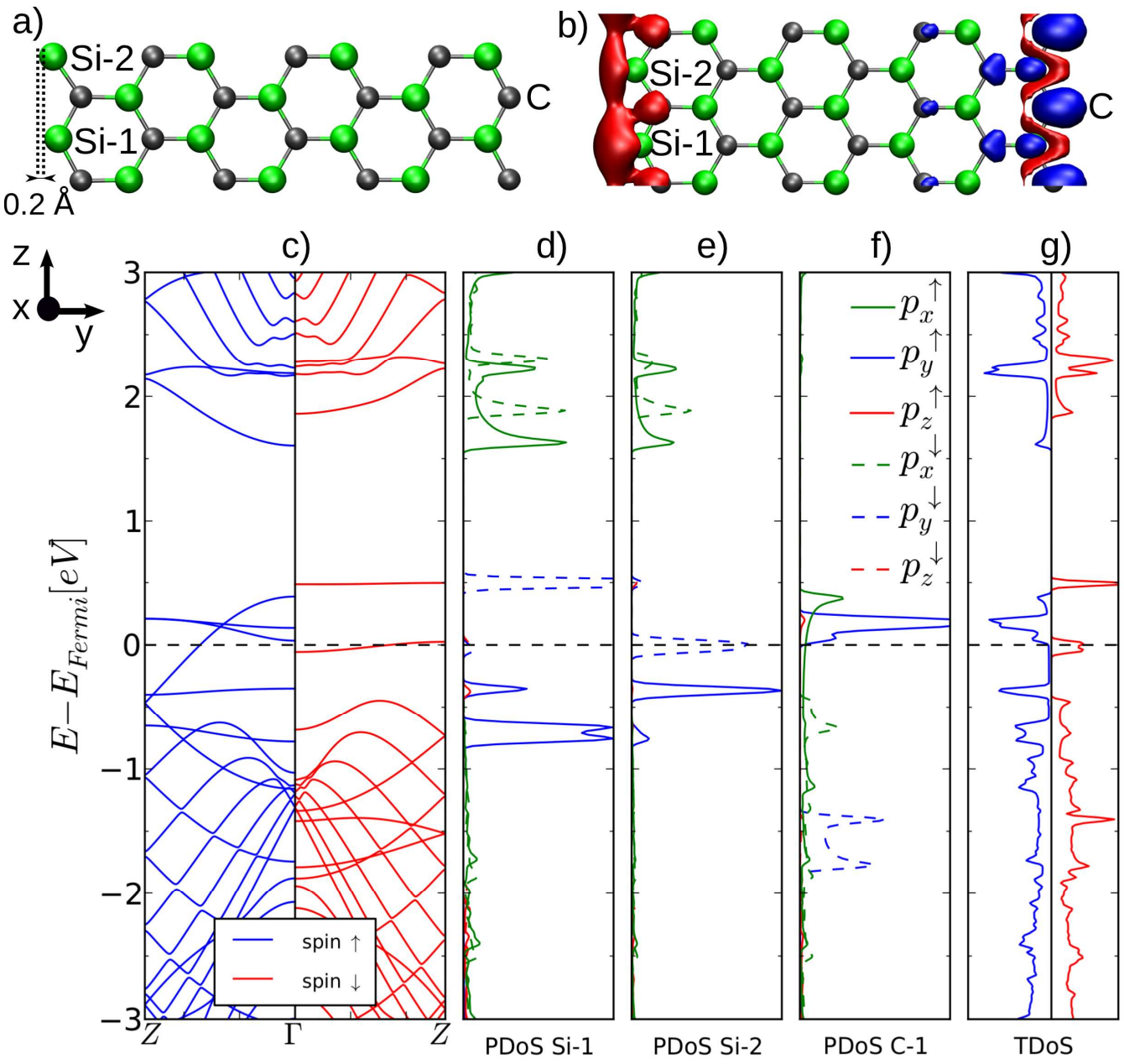

Figure S1. *Fully relaxed unit cell geometry of the bare-edged -[SiC]$_7$-(2) ribbon, of the ground state noted as (↑↑ - ↓↓). Green and gray spheres represent Si and C atoms, respectively. Si atoms are denoted by Si-1 and Si-2 to represent their inequivalency n the Si edge. The relative lateral displacement of the Si atoms by 0.2 Å at the zigzag edge is shown. b) Spin density distribution of the configuration noted as (↑↑ - ↓↓) at an isosurface of 10^{-3} e/Å^3. The blue and red isosurfaces correspond to net spin-up and spin-down electron densities, respectively. c) Spin-resolved band diagram for the spin-up and spin-down states of the -[SiC]$_7$-(2) ribbon. For this ribbon, the projected density of states (PDoS) of Si-1 and Si-2 edge atoms are plotted in d) and e), respectively. f) PDoS is shown for one of the two equivalent C atoms at the opposite. The total density of states (TDoS) of the -[SiC]$_7$-(2) ribbon is plotted in g). Horizontal dashes indicate the Fermi energy level.*

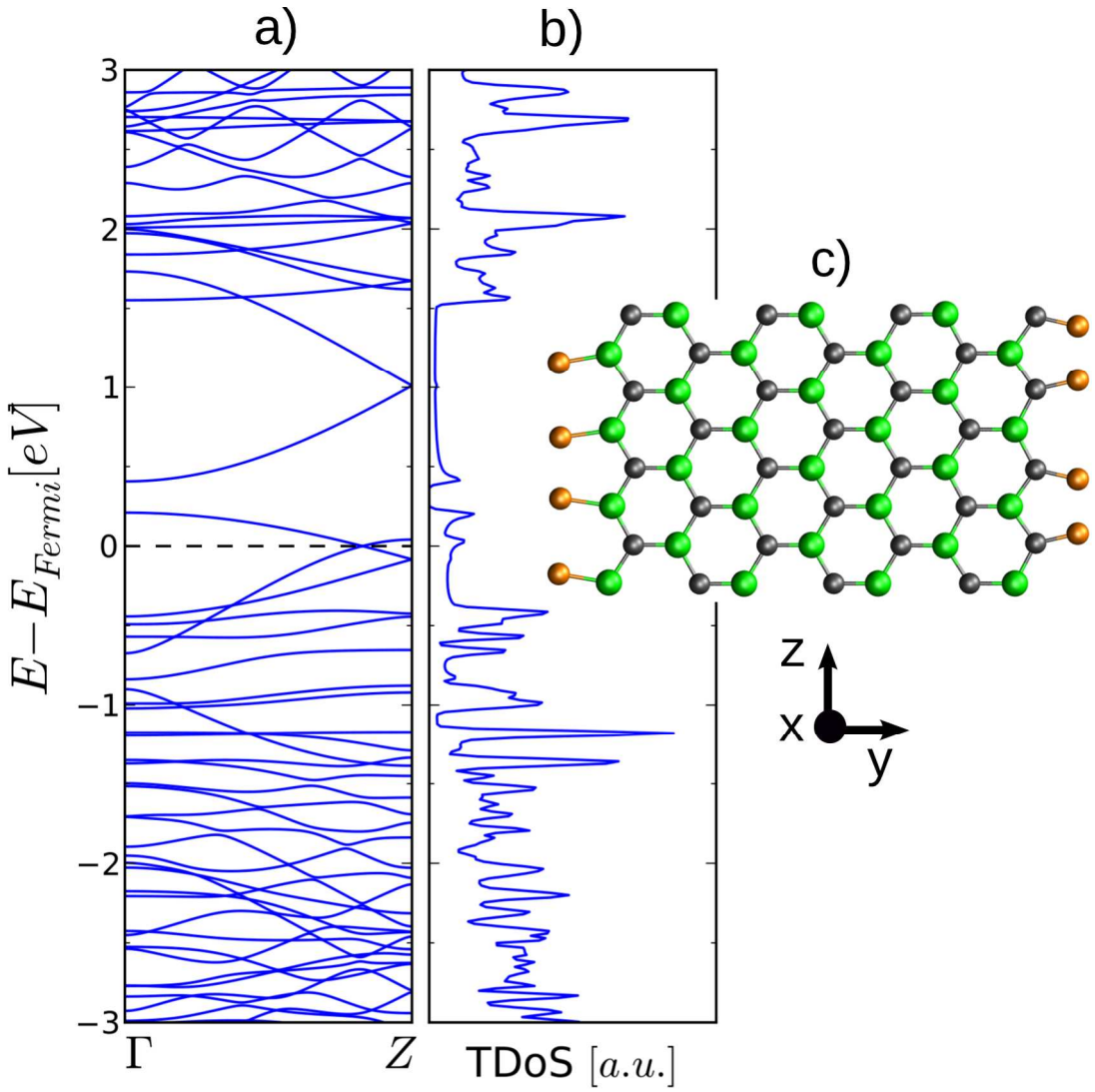

Figure S2. *Electronic band structure and total density of states (TDoS) of a S-[BN]$_7$-S(4) nanoribbon exhibiting a group of four S atoms on the Si edge and two groups of S dimers on the opposite C edge.*