Supporting Information

Tailoring the Electronic and Magnetic Properties of Two-dimensional Silicon Carbide Sheets and Nanoribbons by Fluorination

Zhiming Shi[†,§], Alex Kutana[‡], Guangtao Yu[†], Wei Chen[†], Boris I. Yakobson[‡], Udo Schwingenschlogl *[,§] and Xuri Huang*[,†]

[†] Institute of Theoretical Chemistry, Jilin University, Changchun 130023, People's Republic of China

[‡] Department of Materials Science and NanoEngineering, Department of Chemistry, and the Smalley Institute for Nanoscale Science and Technology, Rice University, Houston, Texas 77005, United States.

[§] King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

* To whom correspondence should be addressed. Email: Udo.Schwingenschlogl@kaust.edu.sa or huangxr@jlu.edu.cn.

Table S1. Bond lengths of 2D-*f*F-chair-SiC obtained for cutoff energies of 360 and 500 eV.

Bond length (Å)	C-Si	C-F	Si-F
360 eV	1.912	1.442	1.605
500 eV	1.912	1.449	1.609

Figure S1. Band structure of 2D-*f*F-chair-SiC obtained for a cutoff energy of 500 eV.

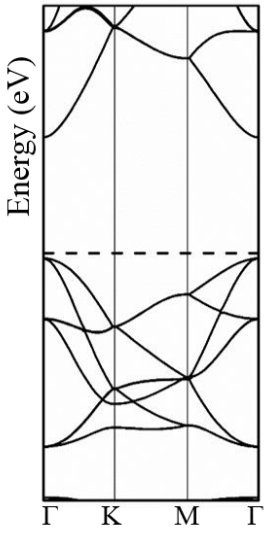

Figure S2. Snapshot of the fully fluorinated SiC sheet in chair conformation at the end of the BOMD calculation.

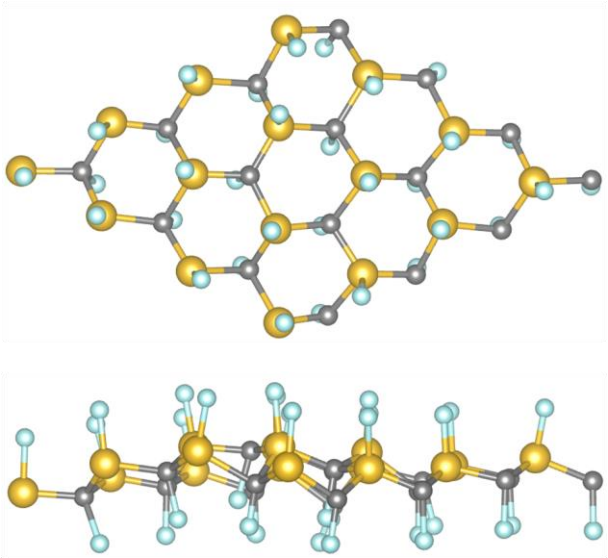

Figure S3. Band structures of 2D-*f*F-boat-SiC (left) and 2D-*f*F-stirrup-SiC (right).

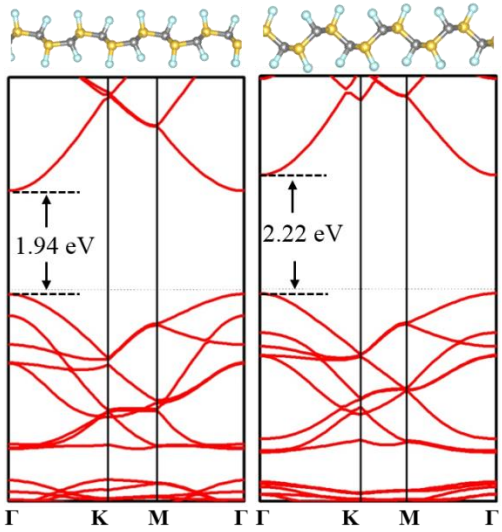

Figure S4. Structural transition with increasing F concentration in the 3×3 supercell. The four ground states are marked by dashed boxes.

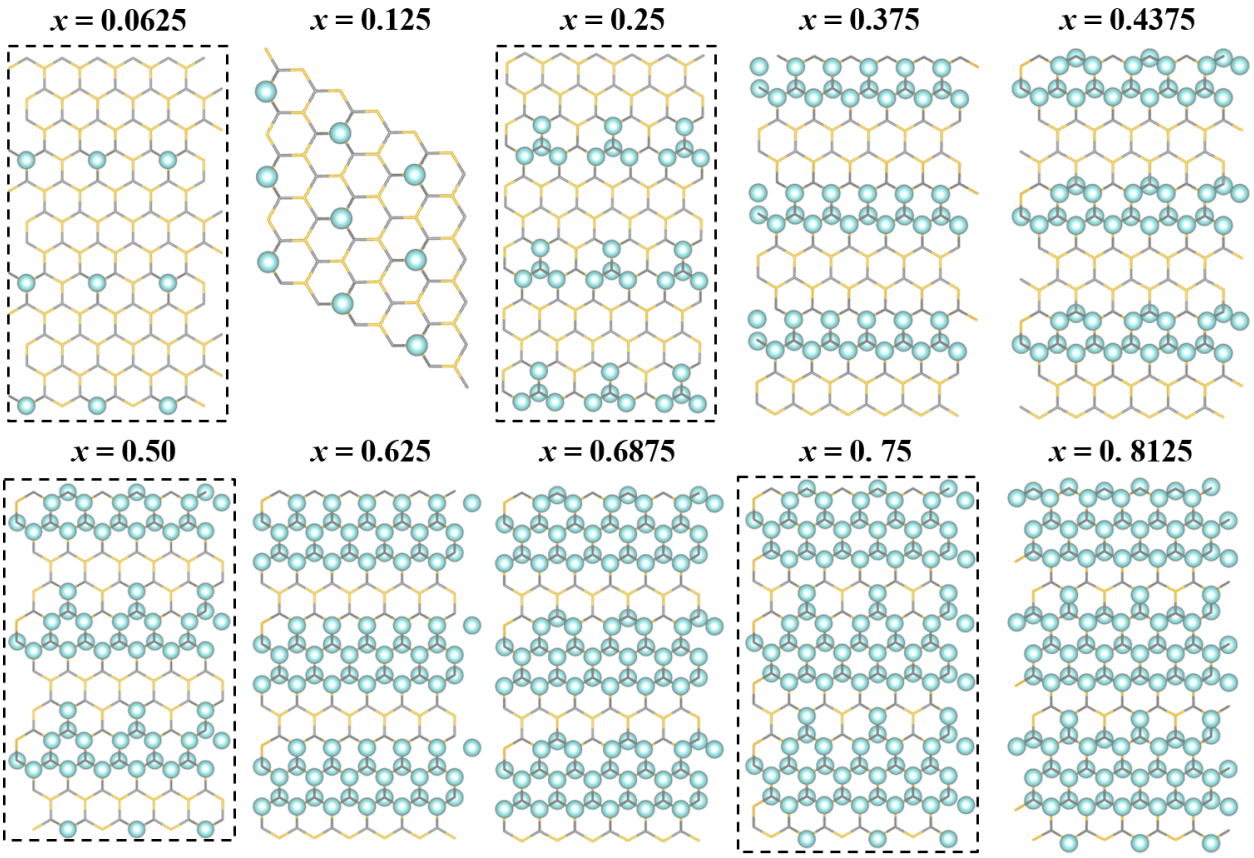

Figure S5. DOSs of the partially fluorinated SiC sheet. Gray shadows show the total DOS, red and blue curves the contributions of the sp^2-C atoms in the spin-up and spin-down channels, respectively.