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Successive hydrogenation starting from the edge(s): an effective approach to fine-tune the electronic and magnetic behaviors of SiC nanoribbons

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(I) Fully hydrogenated zigzag and armchair SiCNRs with different configurations.

Considering that the stirrup configuration is the most stable structure of fully hydrogenated BN single layer against chair and boat,[1] in this work, we have also taken into account these three different conformers to confirm the most stable form of fully hydrogenated zigzag and armchair SiCNRs. With the PW91 functional, 1×1×51 *k*-points, and a 360-eV cutoff, we have performed detailed DFT computations on the sampled fully hydrogenated 8-zSiCNR and 13-aSiCNR (denoted as *f*H-*8*-zSiCNR and *f*H-*13*-aSiCNR), and their fully relaxed structures with chair, boat, and stirrup are illustrated in Figure S1. The computed results reveal that all of these fully hydrogenated SiCNRs present nonmagnetic ground states, and fully hydrogenated zigzag and armchair SiCNRs with chair configuration exhibit much lower energies than those with both boat and stirrup (Table S1), demonstrating that the chair configuration is the most stable form of hydrogenated SiCNRs. Thus, in this work, it has been employed in all of the hydrogenated zigzag and armchair SiCNRs.

1 A. Bhattacharya, S. Bhattacharya, C. Majumder, G. P. Das, *Phys. Status Solidi RRL* 2010, **4**, 368–370.

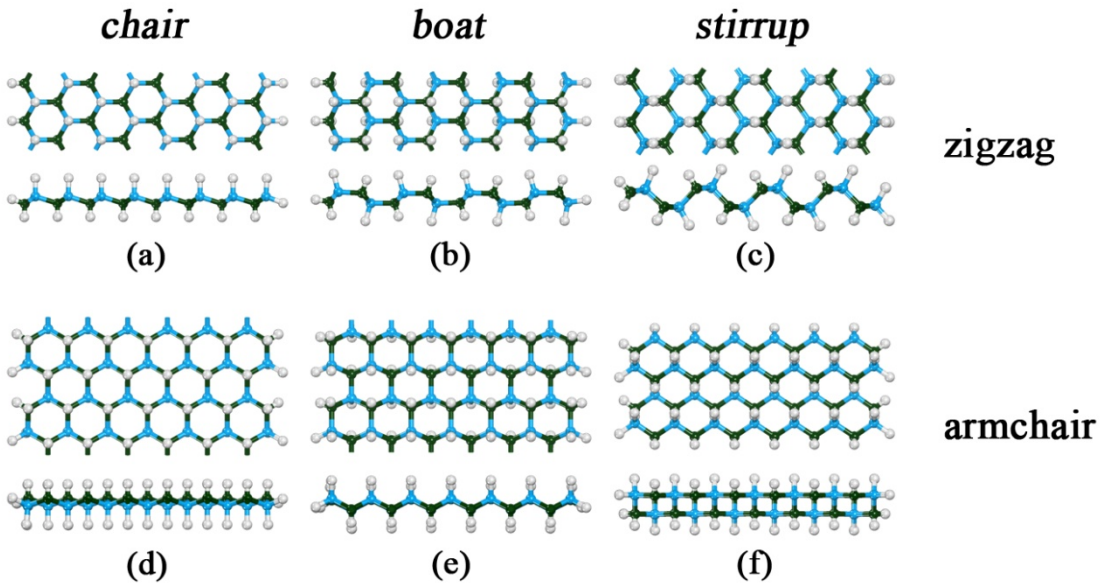

***Figure S1*. Top and side views of the fully relaxed structures of *f*H-*8*-zSiCNR and *f*H-*13*-aSiCNR with chair (a/d), boat (b/e), and stirrup (c/f) configurations, respectively.**

***Table S1*. Relative energies (meV) of *f*H-*8*-zSiCNR and *f*H-*13*-aSiCNR with both boat and stirrup configurations to those with chair.**

Structures	chair	boat	stirrup
*f*H-*8*-zSiCNR	0	504.7	79.5
*f*H-*13*-aSiCNR	0	1003.0	145.9