Supporting Information for

Insertion of Line Defect in Nanoribbons of Graphene, Boron Nitride and Hybrid of them: An AIMD study

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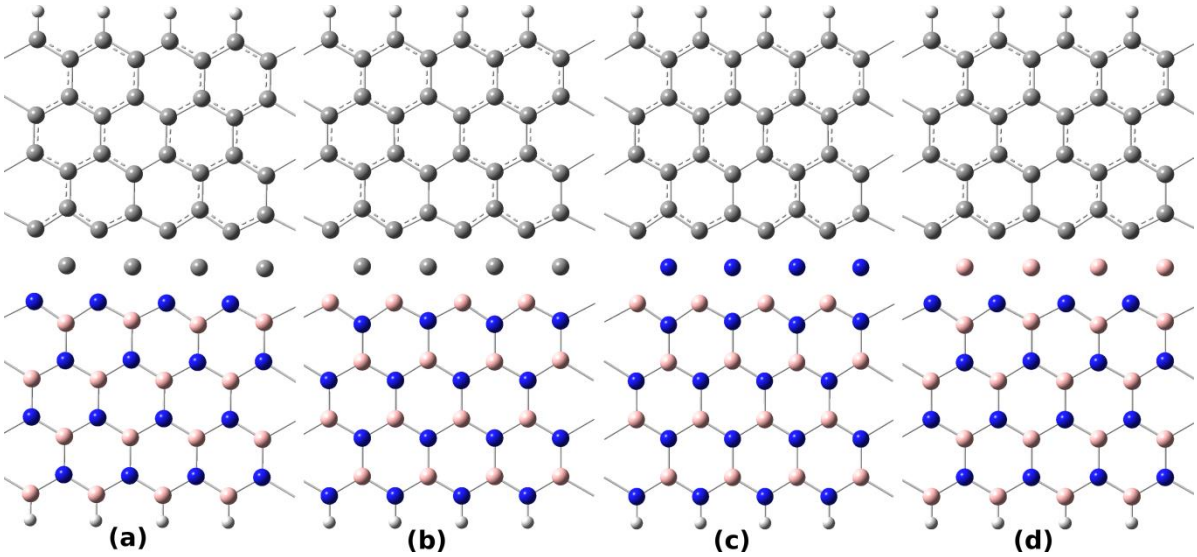

Figure S1. Initial structures of (a) C-ZBNCNR-CB, (b) C-ZBNCNR-CN, (c) N-ZBNCNR-CN and (d) B-ZBNCNR-CB.

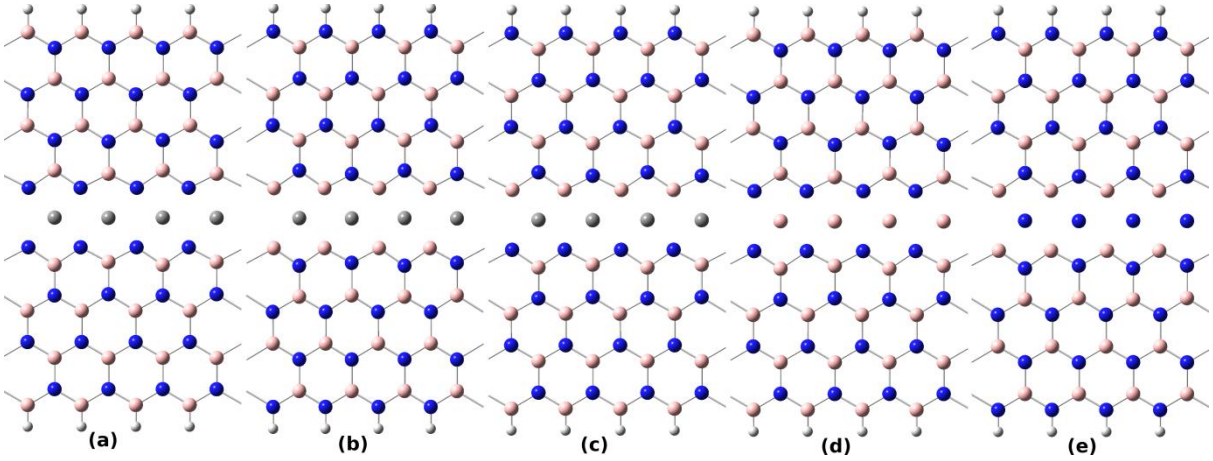

Figure S2. Initial structures of (a) C-ZBNNR-BB, (b) C-ZBNNR-NN, (c) C-ZBNNR-BN, (d) B-ZBNNR-BB and (e) N-ZBNNR-NN.

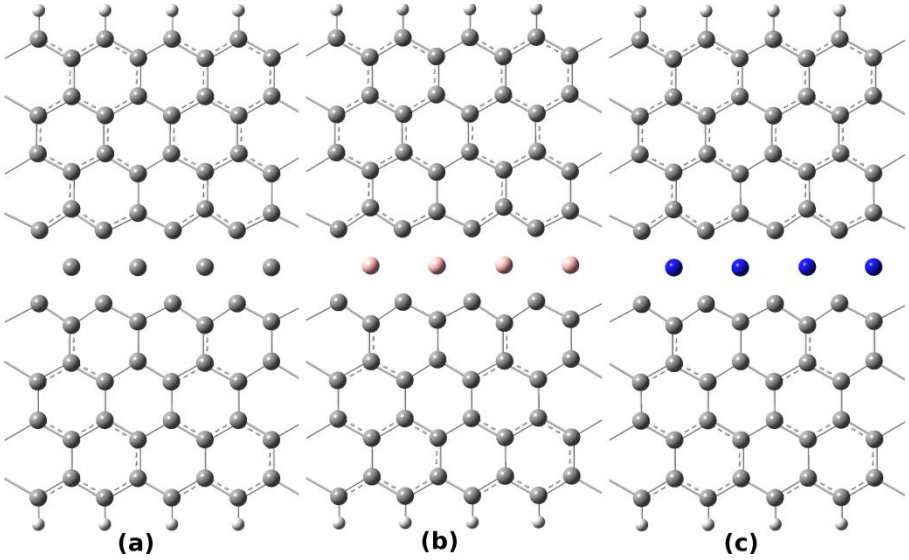

Figure S3. Initial structures of (a) C-ZGNR, (b) B-ZGNR and (c) N-ZGNR.

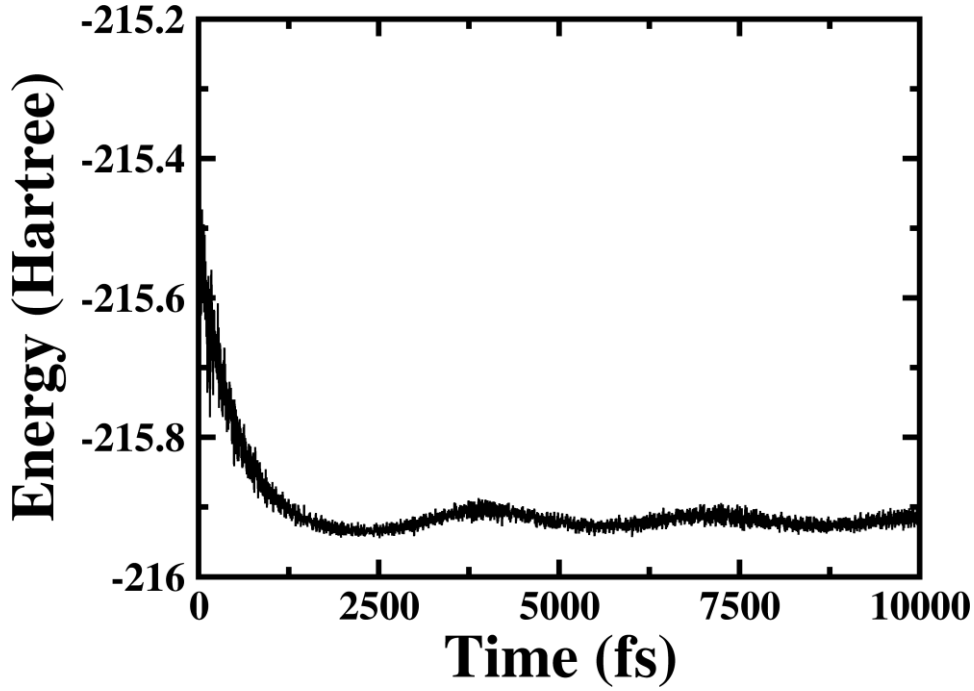

Figure S4. Total energy during 10 ps AIMD simulation for reconstruction of N-ZBNCNR-CN with 300 K and 1 atm pressure.

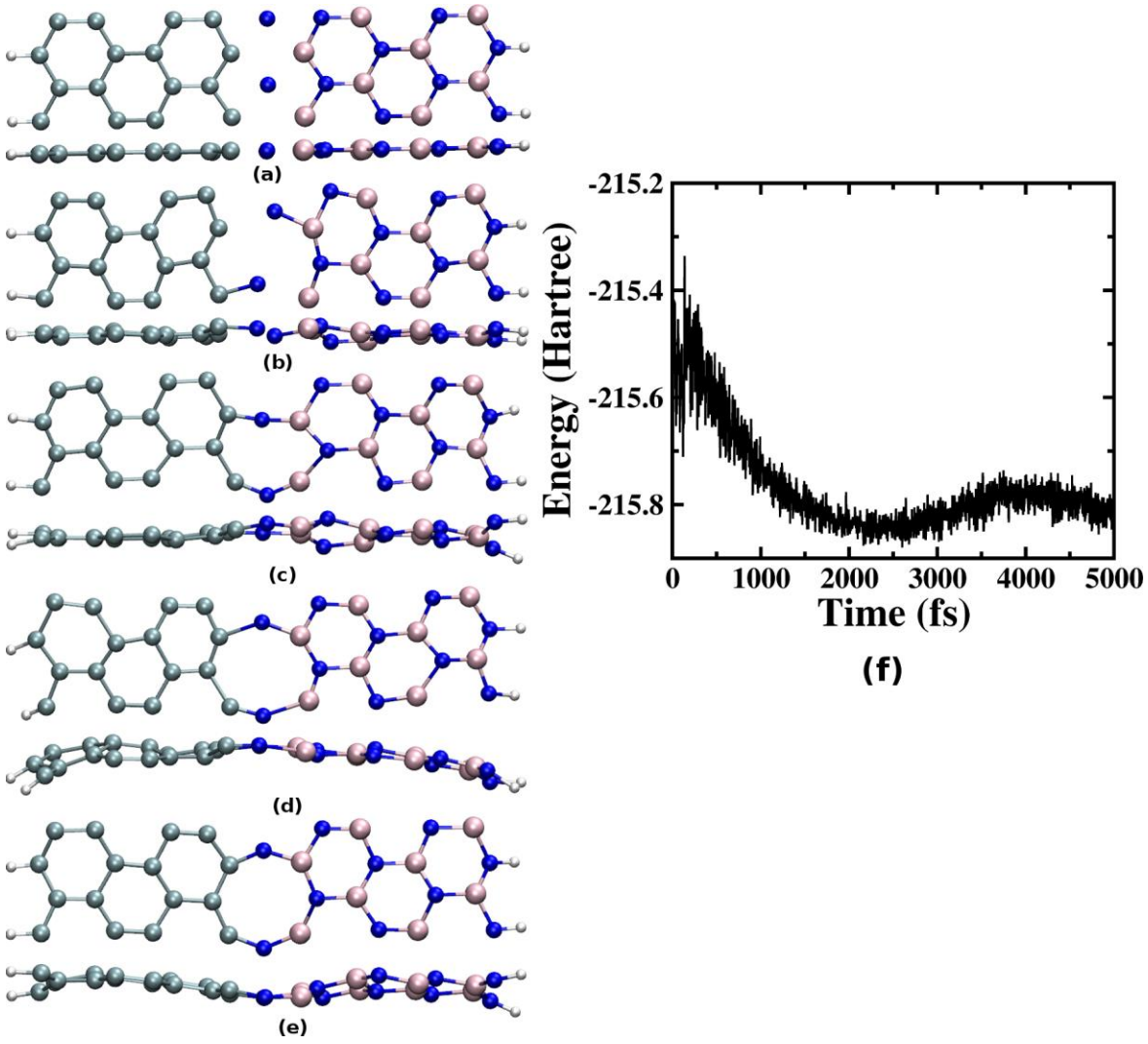

Figure S5. Snapshot from top and side of structurally reconstructed N-ZBNCNR-CN at 1000K after (a) 0.0ps (b) 0.005ps (c) 0.01ps (d) 1ps and (e) 5ps. Deposited N atoms at the grain boundary remain mobile initially (a-c). At around 1ps, grain boundary starts getting reconstructed to 5−8−5 ELD by creating N–N dimer at grain boundary (d). The structure remains unchanged up to 5 ps in this structural form (e). Total energy during 5 ps AIMD simulation is shown in (f).

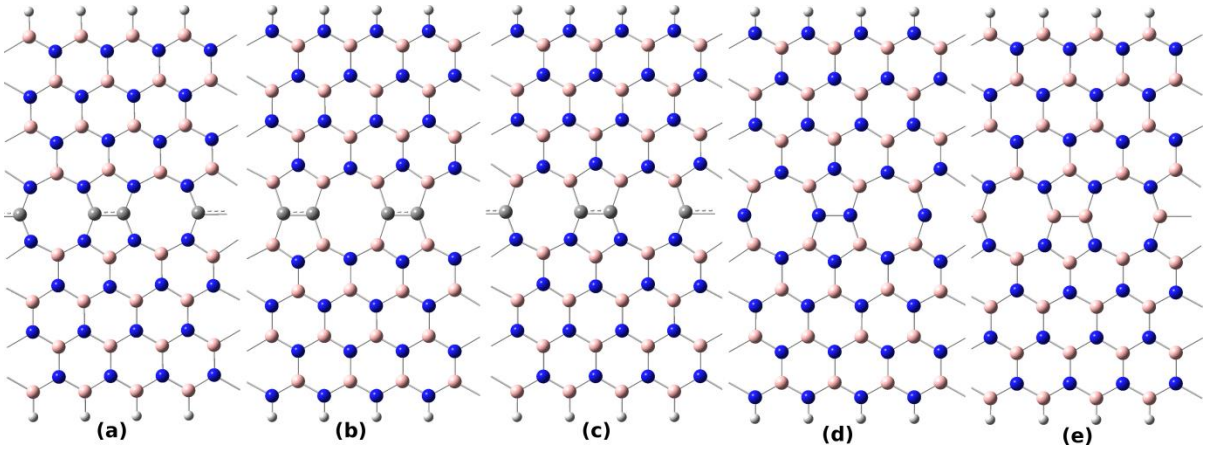

Figure S6. Equilibrated structures of (a) C-ZBNNR-BB, (b) C-ZBNNR-NN, (c) C-ZBNNR-BN (d) B-ZBNNR-BB and (e) N-ZBNNR-NN after performing AIMD simulation at 300K for 5ps.

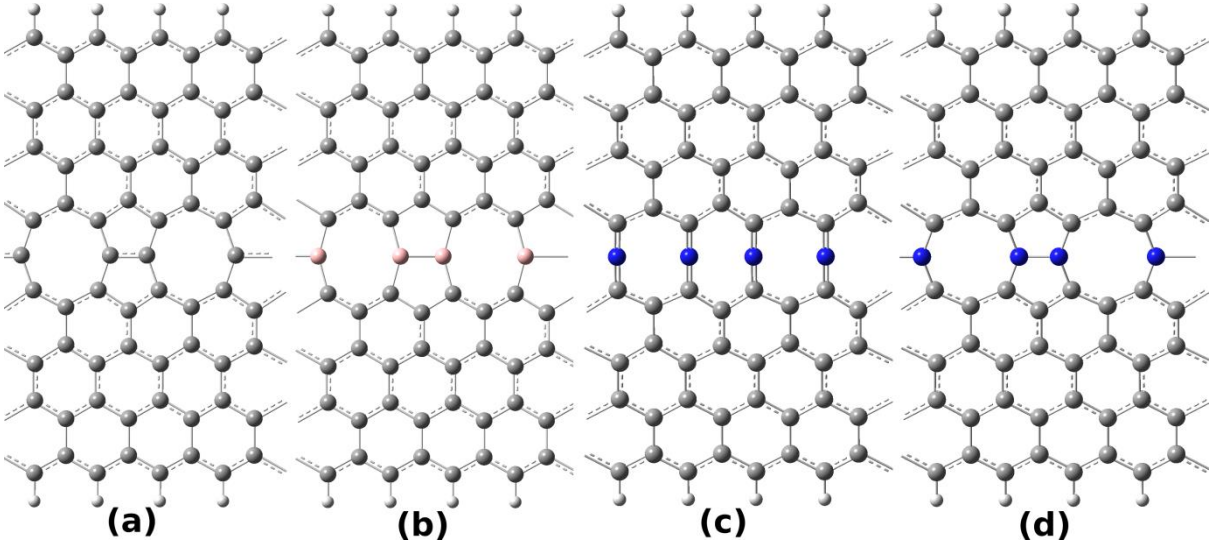

Figure S7. Equilibrated structures of (a) C-ZGNR at 300K, (b) B-ZGNR at 300K, (c) N-ZGNR at 300K (d) N-ZGNR at 1000K after performing AIMD simulation for 5ps.

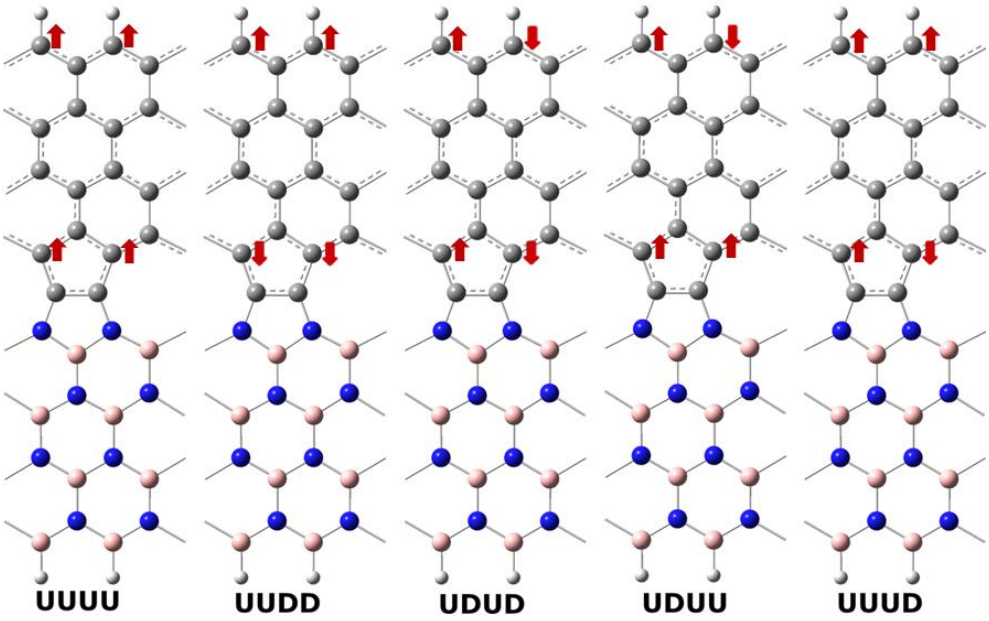

Figure S8. Various Spin configurations and their corresponding name for C-ZBNCNR-CB. Up- and down-spins are denoted are U and D, respectively.

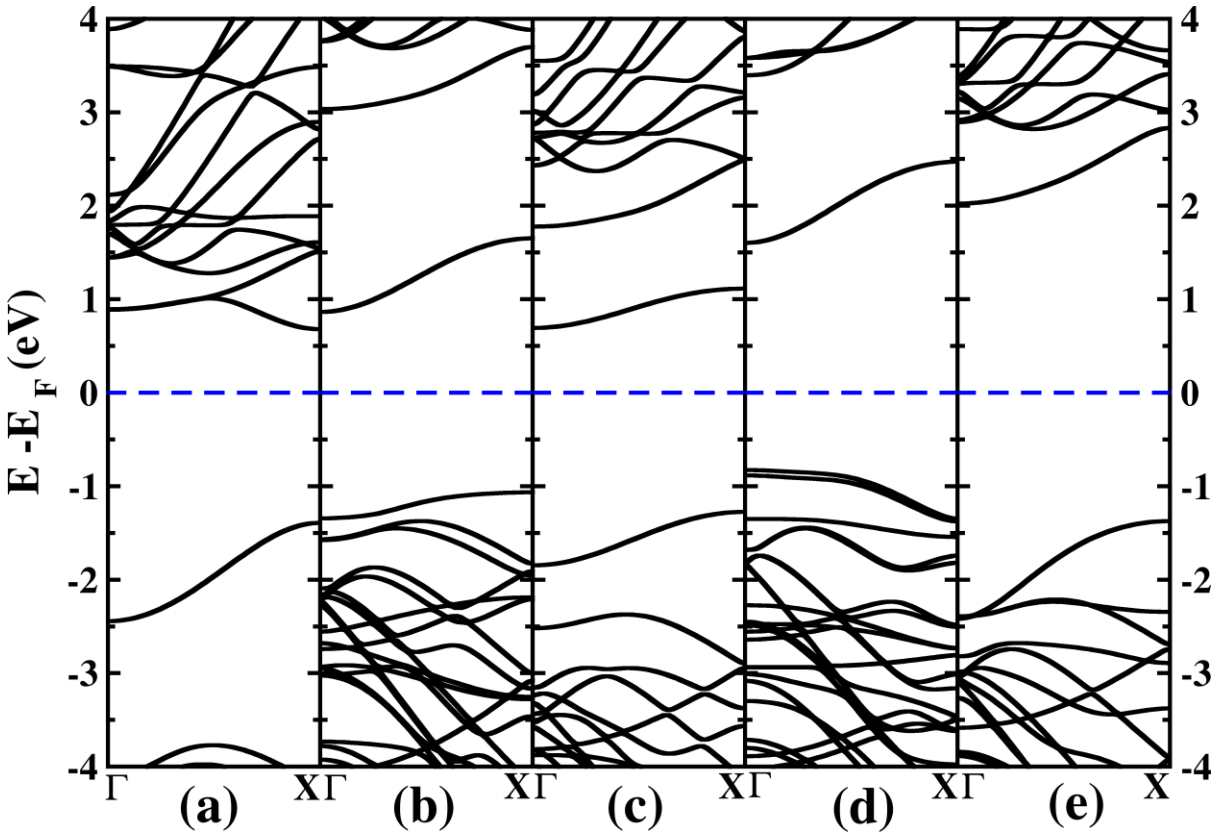

Figure S9. Spin polarized band structure of (a) C-ZBNNR-BB, (b) C-ZBNNR-NN, (c) C-ZBNNR-BN (d) B-ZBNNR-BB and (e) N-ZBNNR-NN.

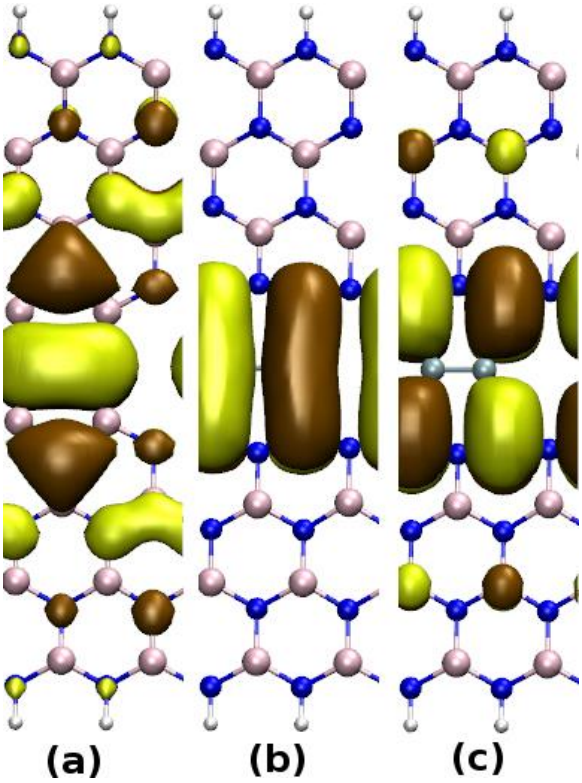

Figure S10. Wave function plot of C-ZBNNR-NN for (a) valance band, (b) conduction band and (c) second conduction band at the Γ-point.

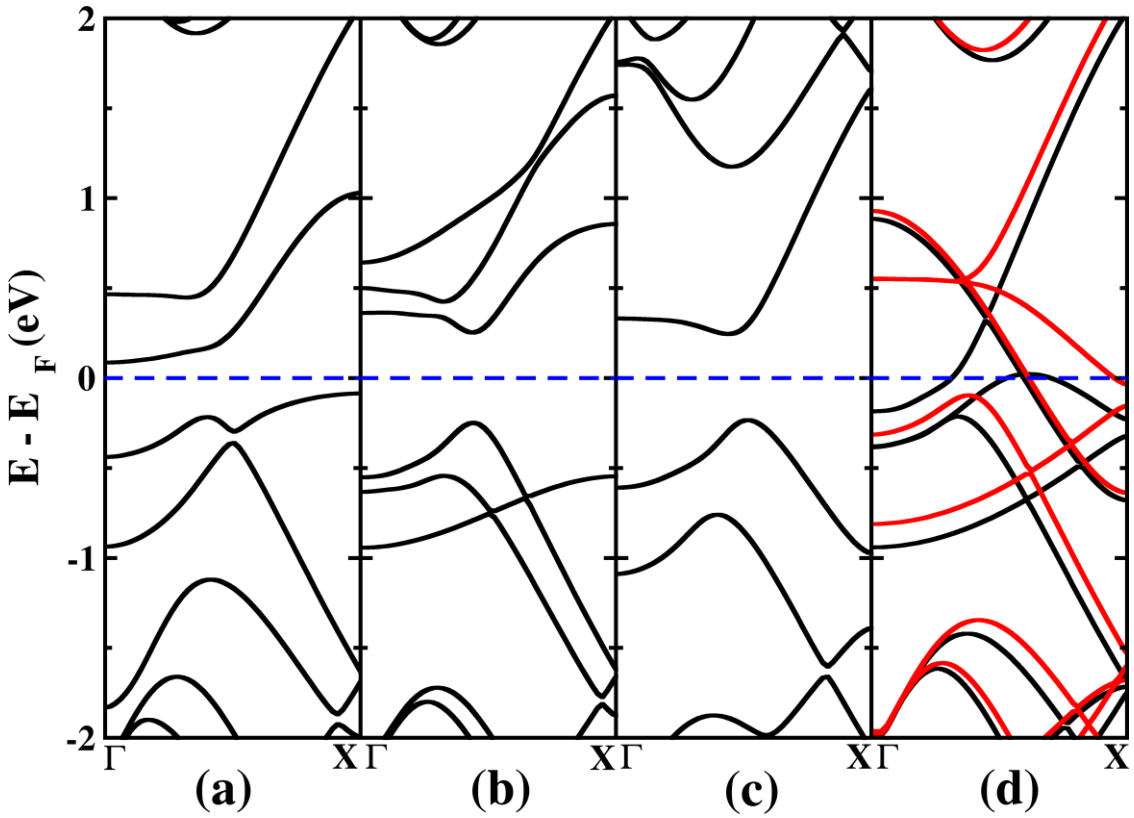

Figure S11. Spin polarized band structure of (a) C-ZGNR, (b) B-ZGNR, (c) N-ZGNR, reconstructed at 1000K i.e. contains 5–8–5 ELD and (d) N-ZGNR, reconstructed at 300K i.e. having 8–8–8 ELD at grain boundary.