

Fig. S1 Total density of states of (a) BeBe-7, (b) BeBe-10, (c) BeN-5, (d) BeN-6, (e) NN-6, and (f)

NN-7 nanoribbons with the NM configurations

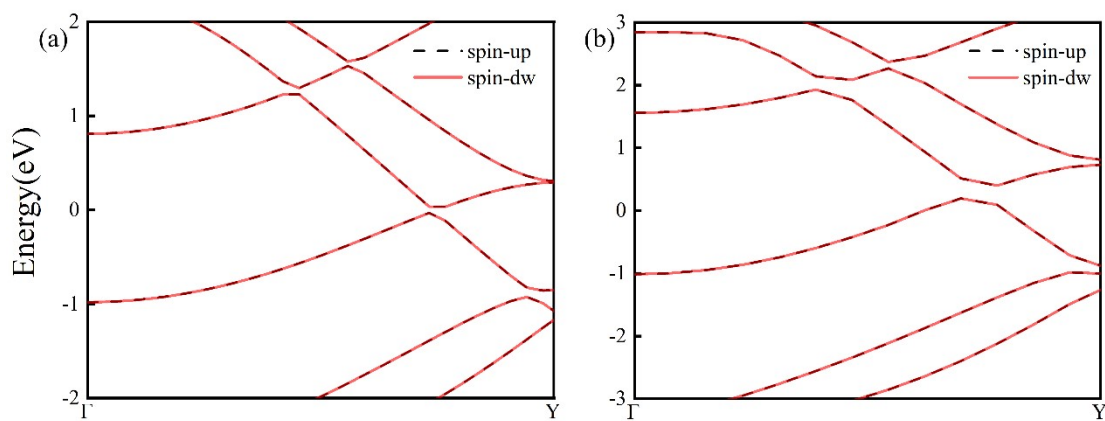


Fig. S2 Band structures of BeBe-7 nanoribbon based on (a) PBE and (b)HSE methods, respectively.

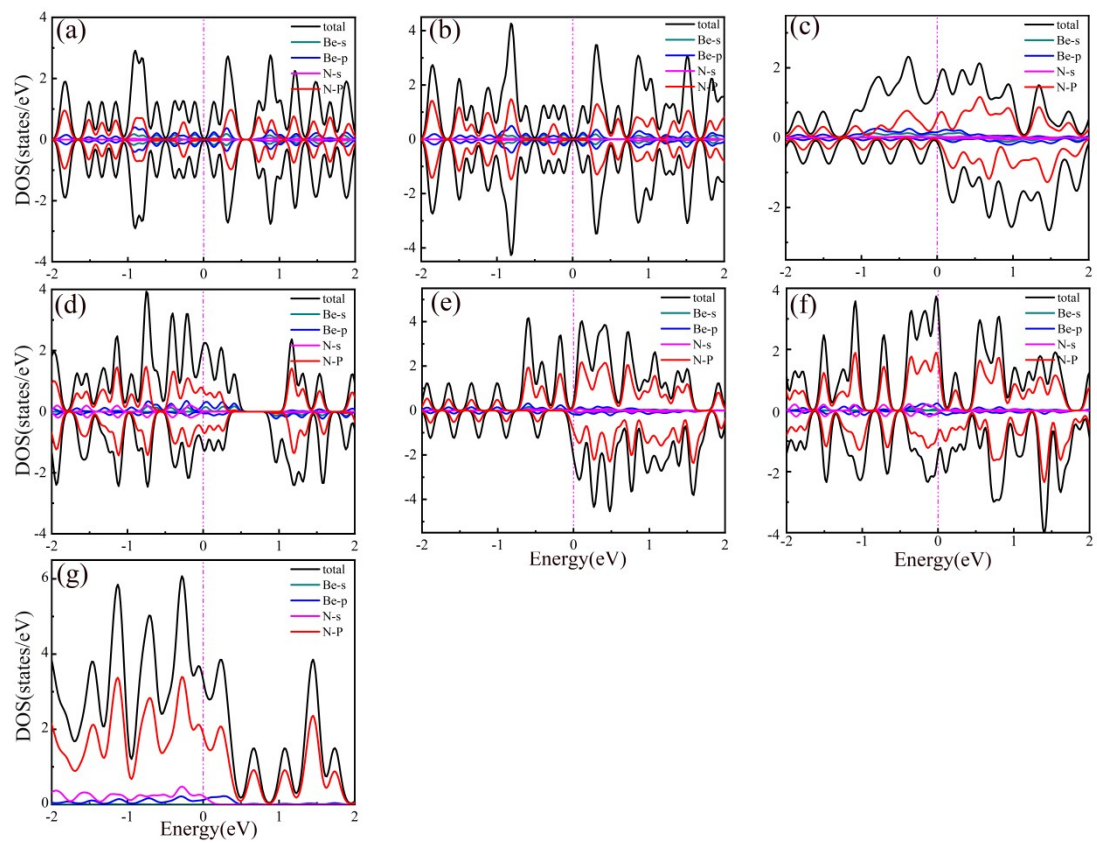


Fig. S3 The total and partial density of states (DOS) in (a) BeBe-7, (b) BeBe-10, (c) BeN-5, (d) BeN-6, (e) NN-6, (f) NN-7 and (g) NN-8 nanoribbons.

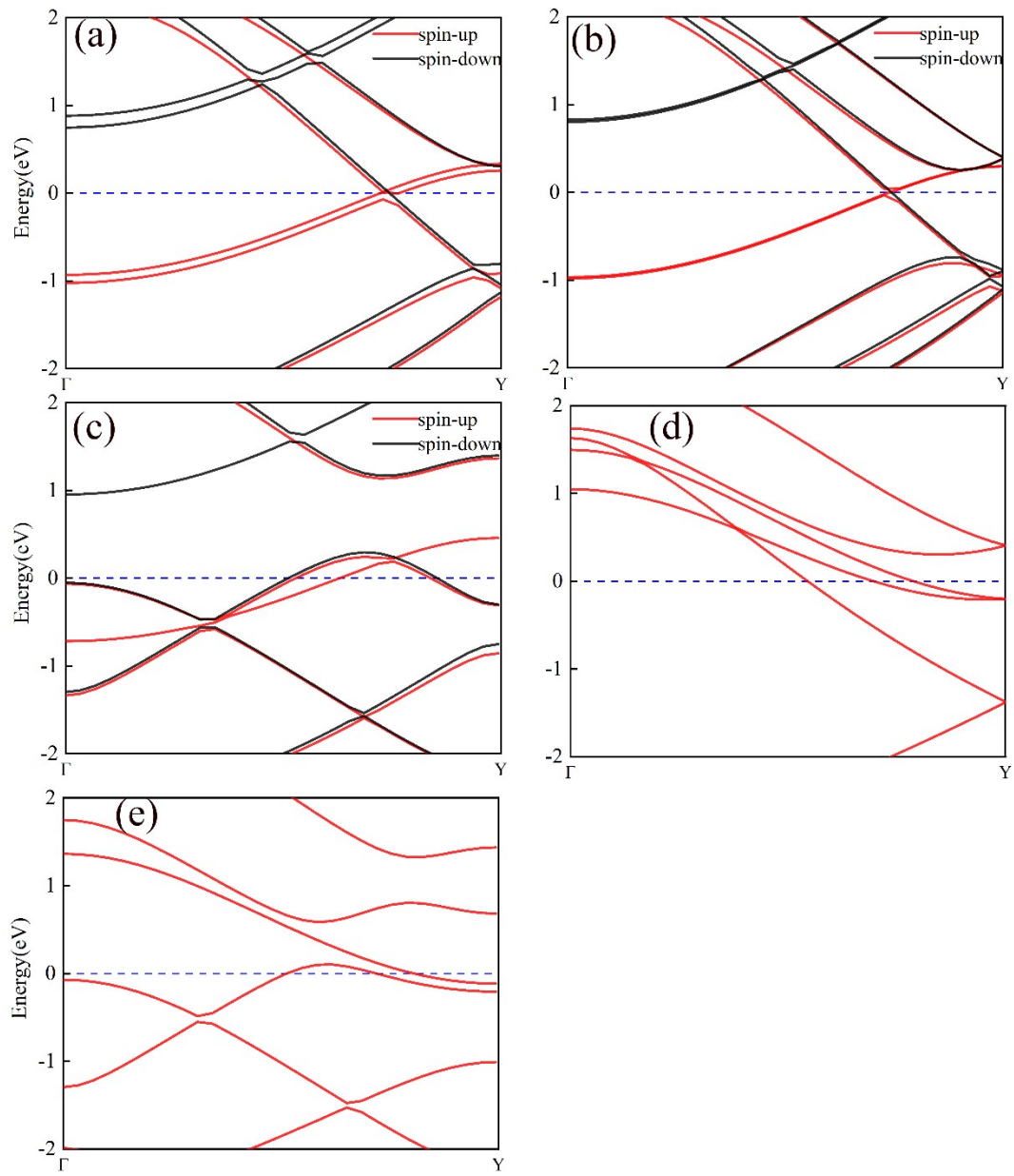


Fig. S4 Band structures of the metastable in (a) BeBe-7(FM), (b) BeBe-10(FM), (c) BeN-6(FM), (d)

NN-6(NM) and (e) NN-7(NM) nanoribbons.

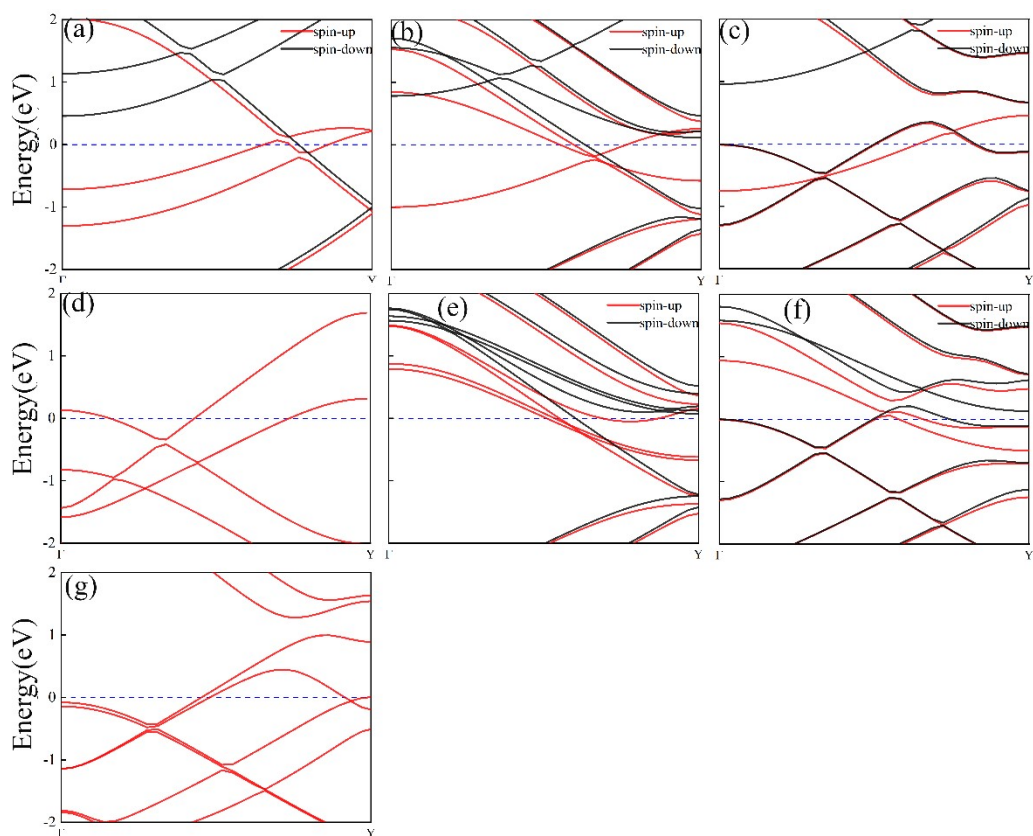


Fig. S5 Band structures of the ground state in (a) BeBe-4, (b) BeN-8, (c) BeN-9, (d) NN-5, (e) NN-9, (f) NN-10 and (g) NN-11 nanoribbons

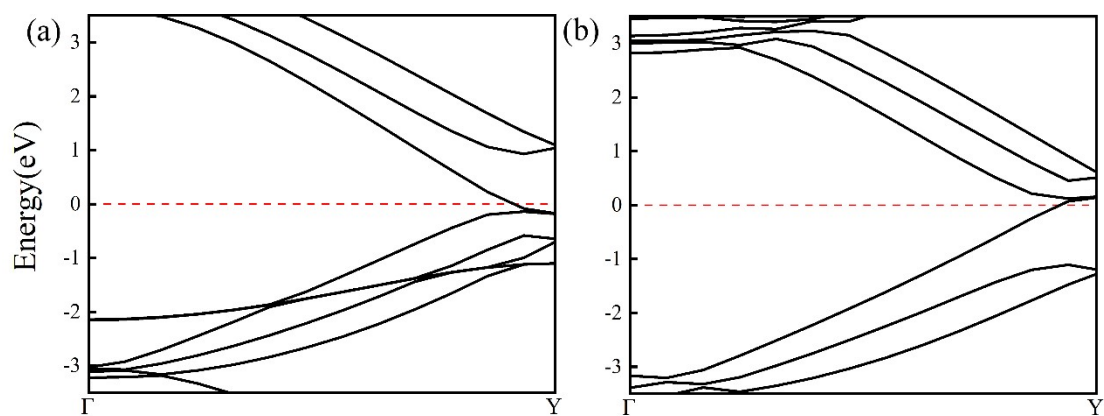


Fig. S6 Band structures of (a) H-BeBe-10 and (b) H-NN-8 nanoribbons by HSE calculation