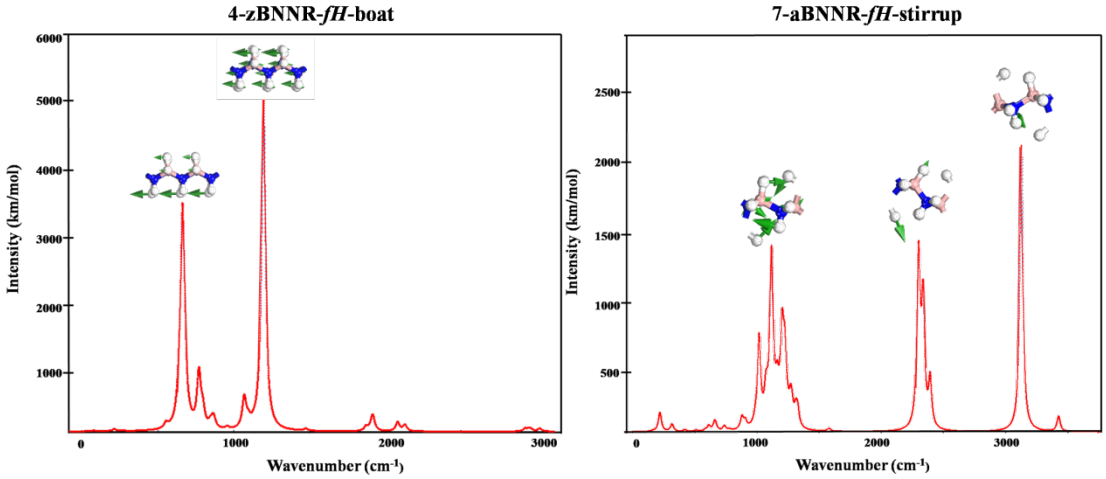
Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

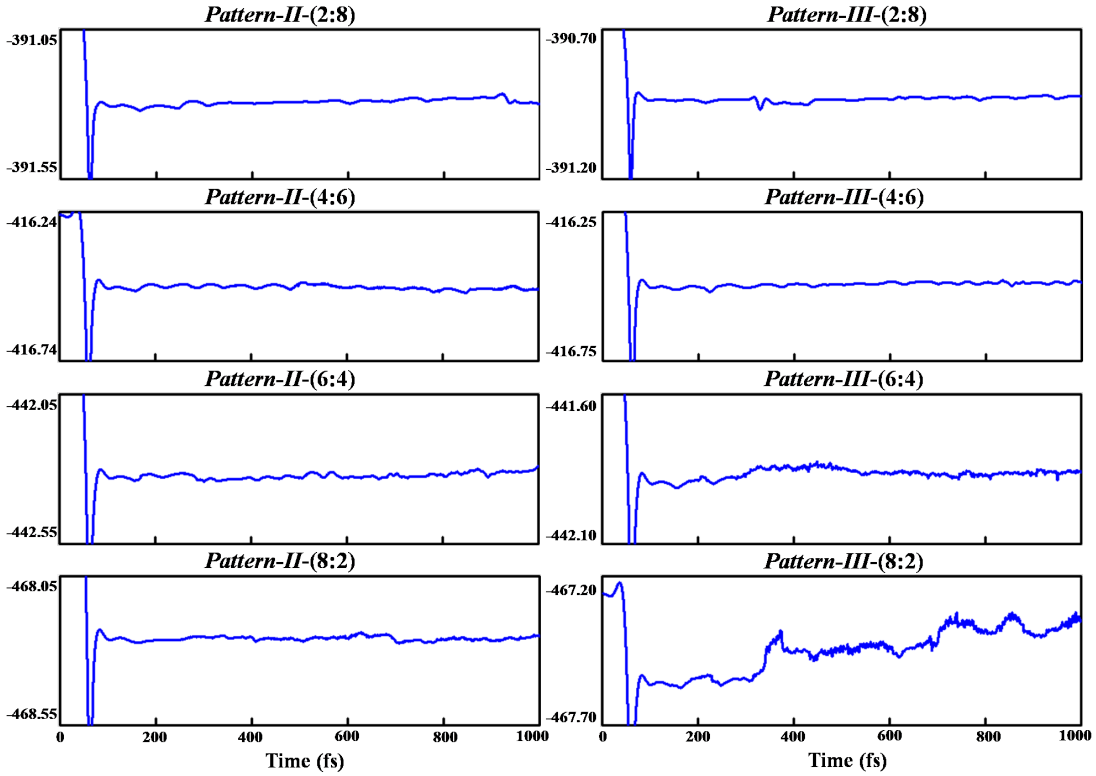
Supplementary Information of the revised manuscript (ID TC-ART-07-2013-031417) "First principles investigation on the stability, magnetic and electronic properties of the fully and partially hydrogenated BN nanoribbons in different conformers"

Figure S1. The vibrational bands and models of the 4-zBNNR-*fH*-boat and 7-aBNNR-*fH*-stirrup.



According to the vibrational bands, no imaginary frequency was found in the both local minima, indicting their great stability. The bending vibrations of B-H bonds, which possessed larger intensity, in 4-zBNNR-*fH*-boat concentrated at 663cm^{-1} and 1198cm^{-1} for B edge and N edge, respectively. The corresponding vibrational models in 7-aBNNRs-*fH*-stirrup concentrated in 1115cm^{-1}, and the stretching vibrations for B-H and N-H bonds also exhibited large intensity at 2302 and 3127cm^{-1}, respectively.

Figure S2. Changes energy with time obtained from molecular dynamics simulation of partially hydrogenated zBNNRs with (a) different patterns and (b) various hydrogenated ratios for *Pattern-II* and *Pattern-III*.



The energy fluctuated around balance positions, suggesting that the partially hydrogenated zBNNRs with different hydrogenated ratios were all stable in *Pattern-II* and *Pattern-III*.