

Supplementary materials

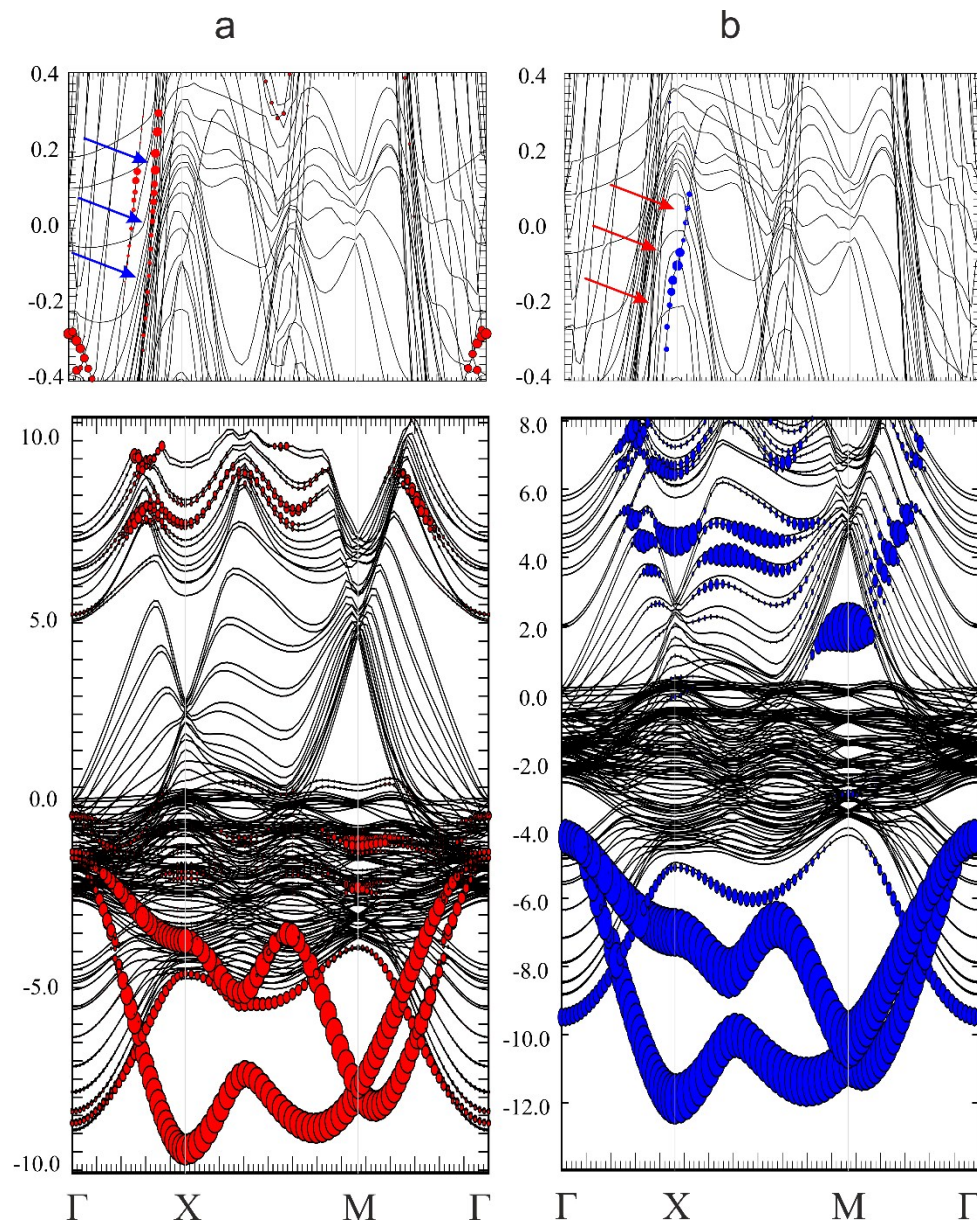


Figure S1: Band structures of *top*:N/*fcc*:BH and *top*:N/*fcc*:B configurations of *h*-BNH/Ni(111) (A) and *h*-BN/Ni(111) (B) heterostructures, respectively. On the top of the figures the details of band structures in the vicinities of the Fermi levels are presented with the same energy scales. On the bottom the wide energy regions are presented. The diameters of the dots reflect partial density of states of *h*-BNH (in red) and *h*-BN (in blue) fragments.

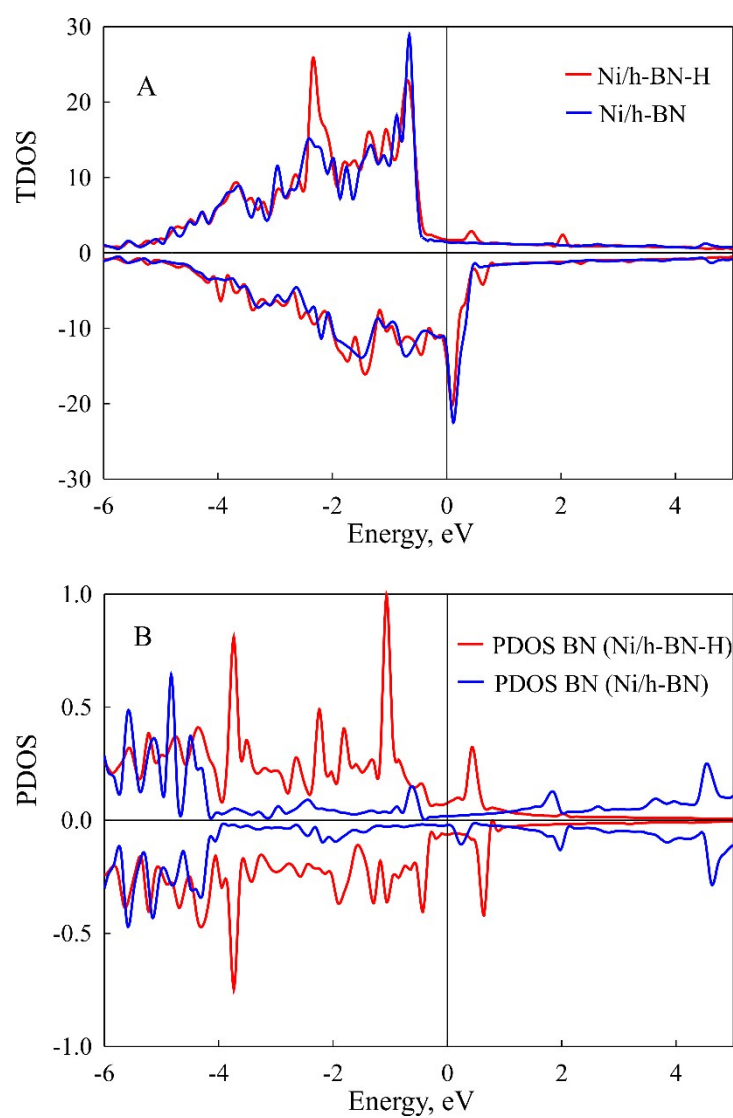


Figure S2: Total (A) and partial (B) density of states of $top:N/fcc:BH$ and $top:N/fcc:B$ configurations of $h\text{-BNH}/\text{Ni}(111)$ (in red) and $h\text{-BN}/\text{Ni}(111)$ (in blue) heterostructures, respectively.