

Supporting Information

Is hexagonal boron nitride always good as a substrate for carbon nanotube-based devices?

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S1. ELECTRONIC BAND STRUCTURES AND EFFECTIVE MASSES

To check whether the electronic properties of a (10,0) CNT would change under various conditions, we calculated the band structures along Γ to A in the 1D Brillouin zone of all the equilibrium configurations we considered and showed in Fig. S1, Fig. S2, and Fig. S3.

For each configuration, we evaluated the effective mass at the bottom of the conduction band of the CNT at Γ point indicated by the black arrow in each figure. The calculated effective masses are listed in Table S1. They seem independent of conditions considered.

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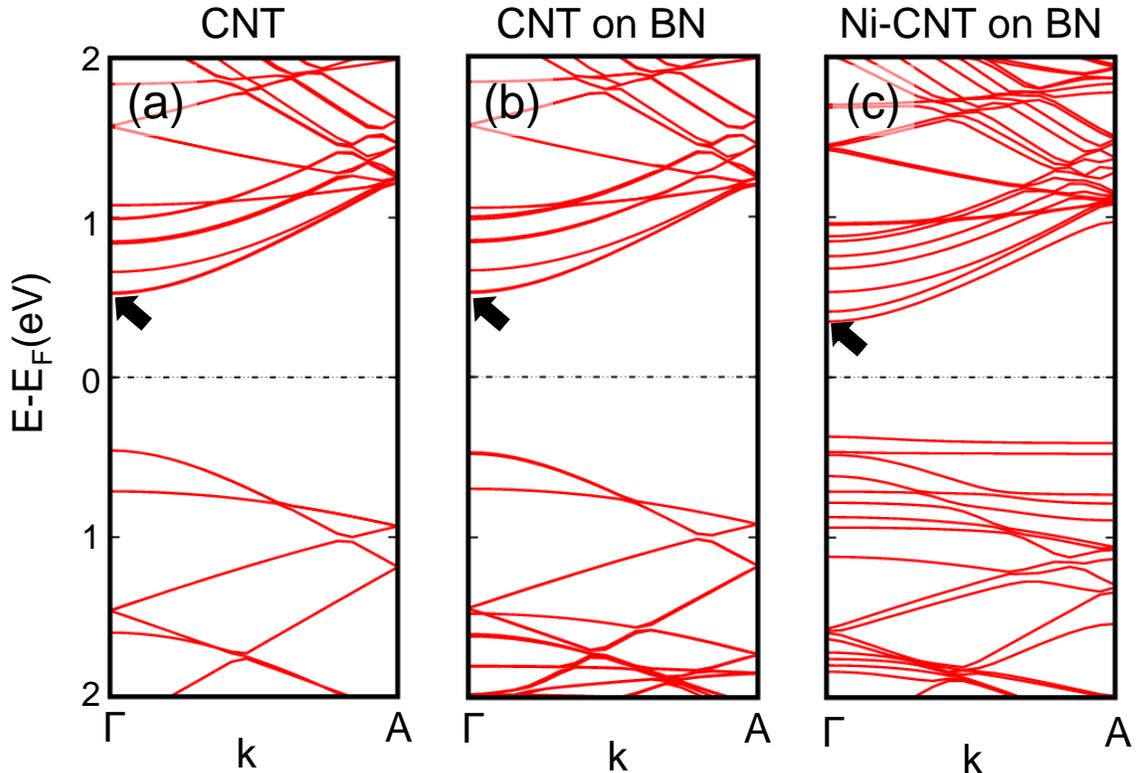


FIG. S1. (Color online) Electronic band structure $E(k)$ along the axial direction Γ - A of a pristine (10,0) CNT (a), a (10,0) CNT on a hBN substrate (b) and (10,0) CNT with a nickel impurity on hBN substrate (c). The black arrow in each graph indicates where the corresponding effective mass was evaluated.

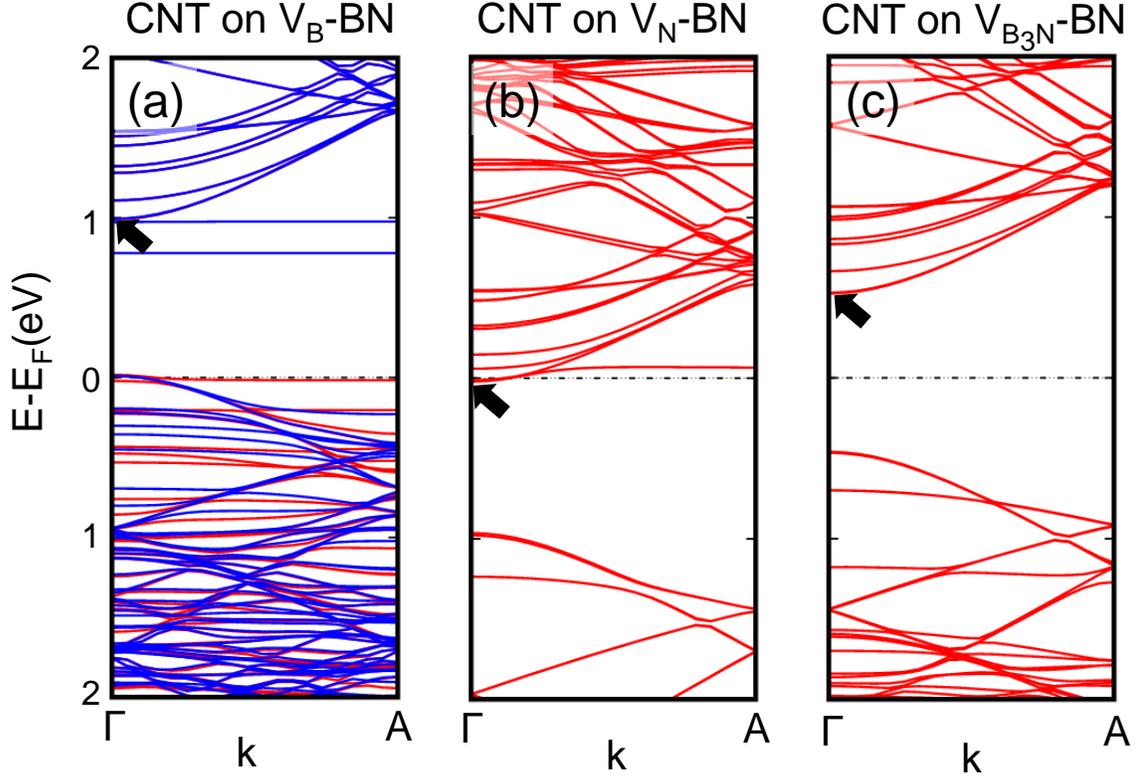


FIG. S2. (Color online) Electronic band structure $E(k)$ along the axial direction Γ -A of a $(10,0)$ CNT on a hBN substrate with a B monovacancy (V_B) (a), a N monovacancy (V_N) (b), and a B_3N triangular multivacancy (c). Red and blue lines represent majority and minority spin, respectively. Black arrow indicates the band at which the effective mass was calculated.

TABLE S1. Effective mass of a CNT under various conditions, evaluated at the bottom of its conduction band at Γ point as shown in Fig. S1, Fig. S2, and Fig. S3.

	Effective mass (m_e^*/m_e)		
	(a)	(b)	(c)
Fig. S1	0.201	0.205	0.194
Fig. S2	0.221	0.247	0.203
Fig. S3	0.209	0.215	0.203

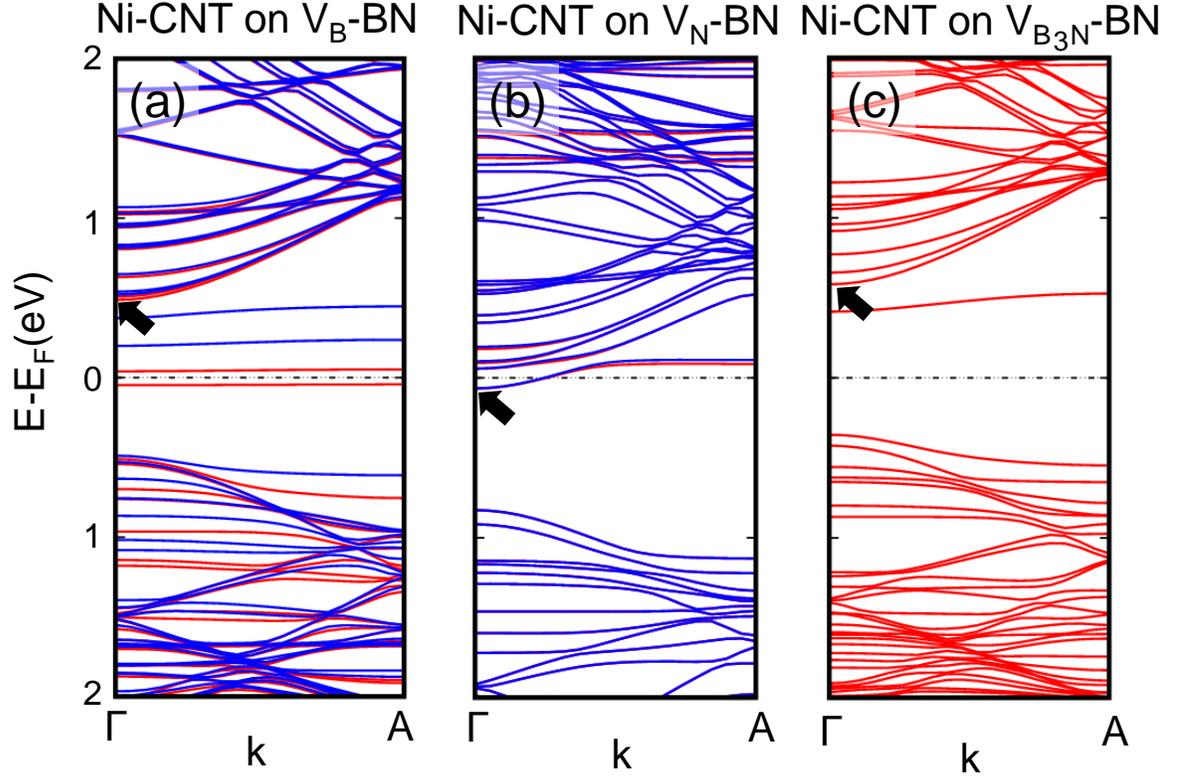


FIG. S3. (Color online) Electronic band structure $E(k)$ along the axial direction Γ -A of a $(10,0)$ CNT with a Ni impurity on a hBN substrate with a B monovacancy (V_B) (a), a N monovacancy (V_N) (b), and a B_3N triangular multivacancy (c). Red and blue lines represent majority and minority spin, respectively. Black arrow indicates the band at which the effective mass was calculated.