

Electronic Supplementary Material

Freestanding χ_3 -Borophene Nanoribbons: A Density Functional Theory Investigation

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Fig. S1: (a) The electron density, (b) the electron localized function with isovalue equal to 0.9, (c) the transmission pathway (at zero energy, and threshold of transmission pathway's weight is equal to 0.2. The scalar bar for the weight of transmission pathway's arrows is shown in Fig.3) of $12XBNR$. (the dashed rectangle shows the unit cell of the ribbon).

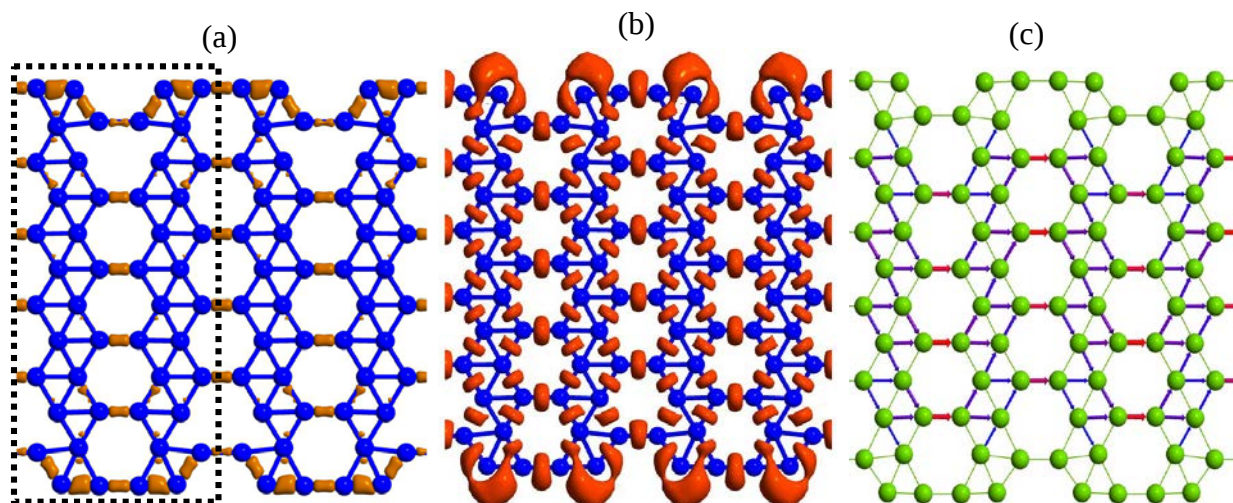


Fig. S1

Fig. S2: (a), (b) and (c) left to right: the electron density, the spin density, the transmission pathway of spin-up electrons, the transmission pathway of spin-down electrons, and the transmission coefficients versus energy of $26aaYBNR$ in FM configuration, AFM configuration, and $26bdYBNR$, respectively. (d) left to right: the electron density, the electron localized function, the transmission pathway of electrons, and the transmission coefficient of $26ccYBNR$. The parameters are similar to the ones in Fig.4.

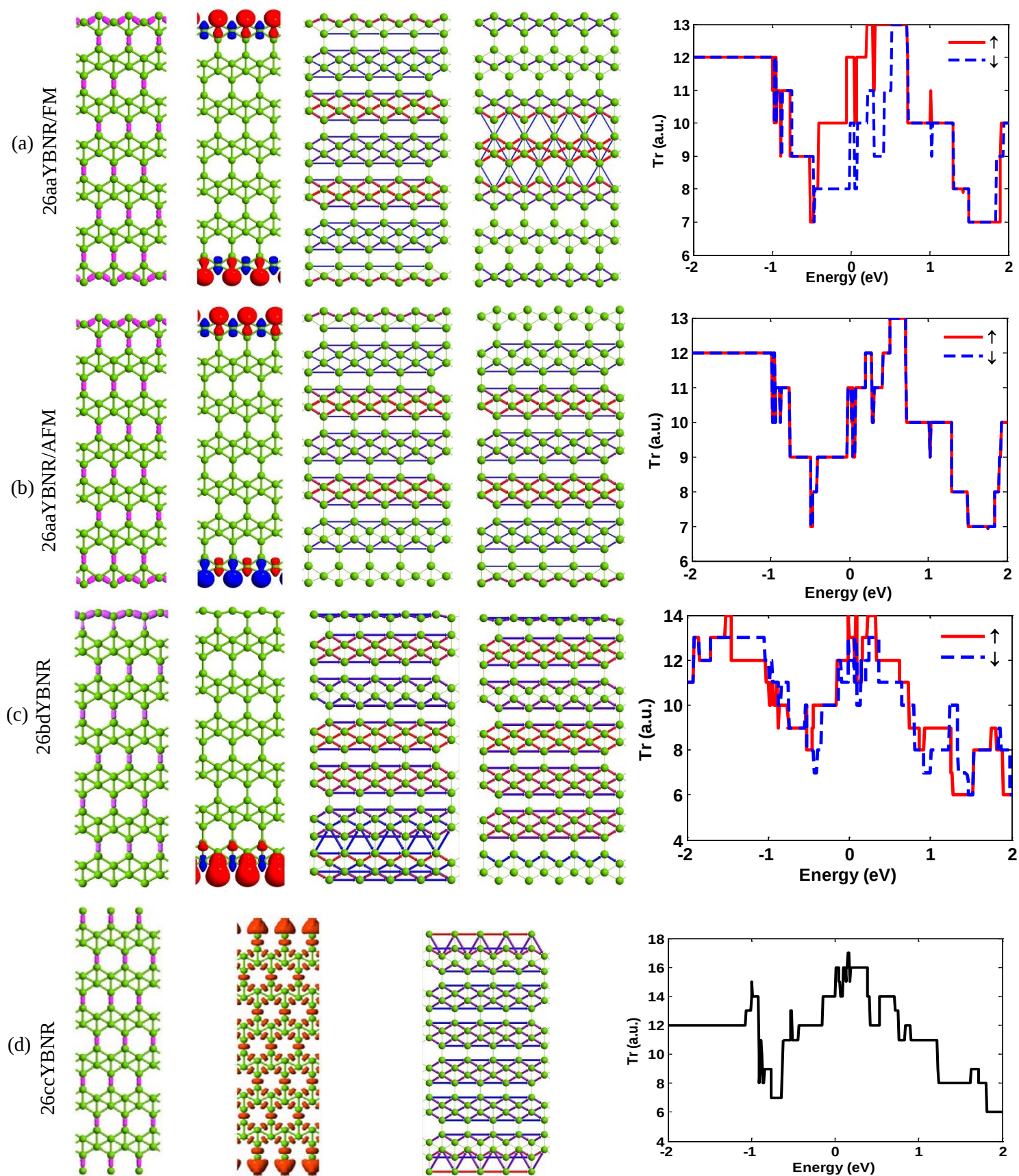


Fig. S2

Fig. S3: (a) and (b) Left to right: the electron density, the spin density, the transmission pathway of spin-up electrons, the transmission pathway of spin-down electrons, and the transmission coefficients versus energy of 27abYBNR in FM configuration and AFM configuration, respectively. (c) Left to right: the electron density, the electron localized function, the transmission pathway of electrons, and the transmission coefficient of 27cdYBNR. The parameters are similar to the ones in Fig.4.

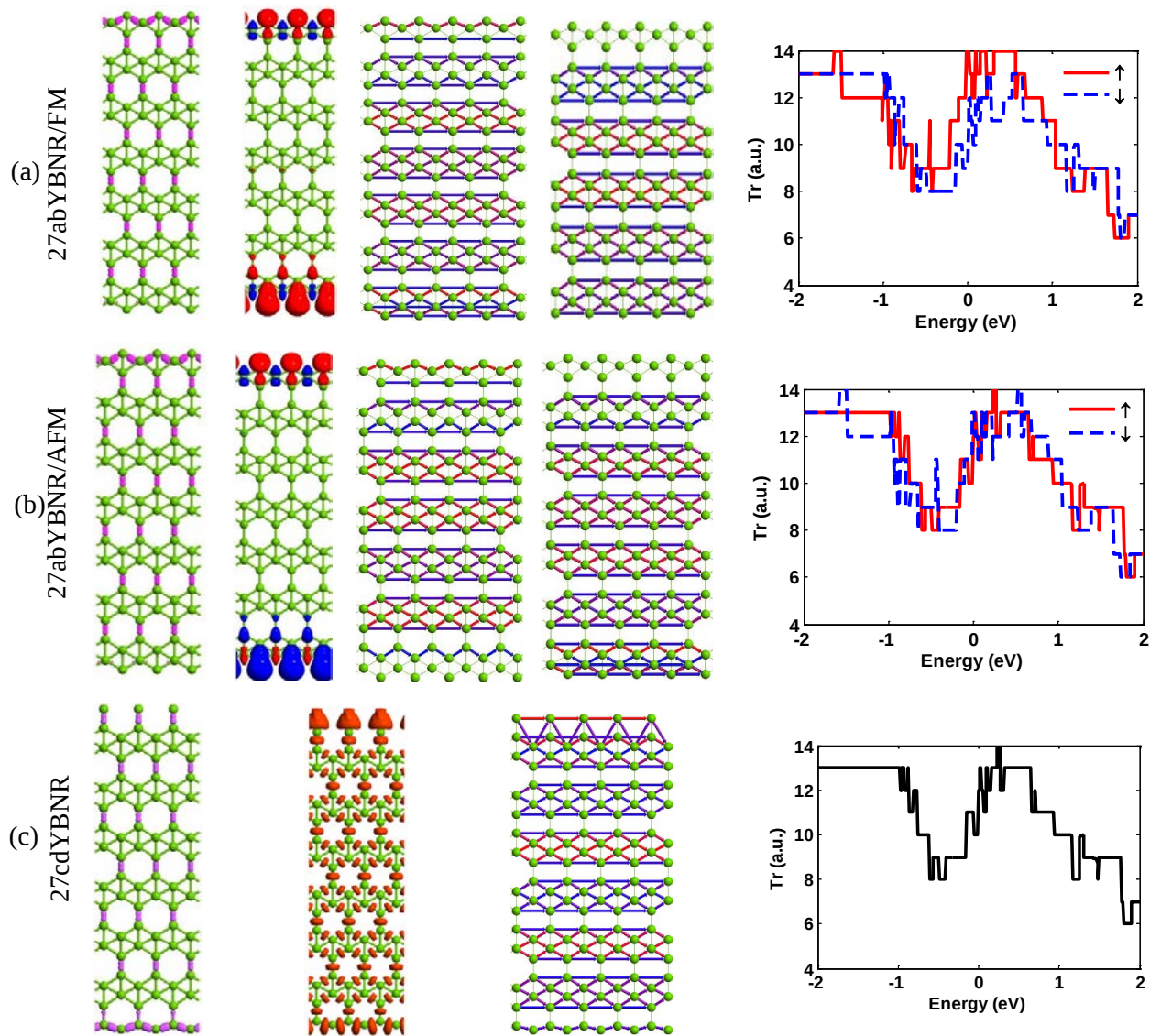


Fig. S3

Fig. S4: (a), (b) and (c) Left to right: the electron density, the spin density, the transmission pathway of spin-up electrons, the transmission pathway of spin-down electrons, and the transmission coefficients versus energy of *28bbYBNR* in FM configuration, AFM configuration, and *28acYBNR*. (d) Left to right: the electron density, the electron localized function, the transmission pathway of electrons, and the transmission coefficient of *28ddYBNR*. The parameters are similar to the ones in Fig.4.

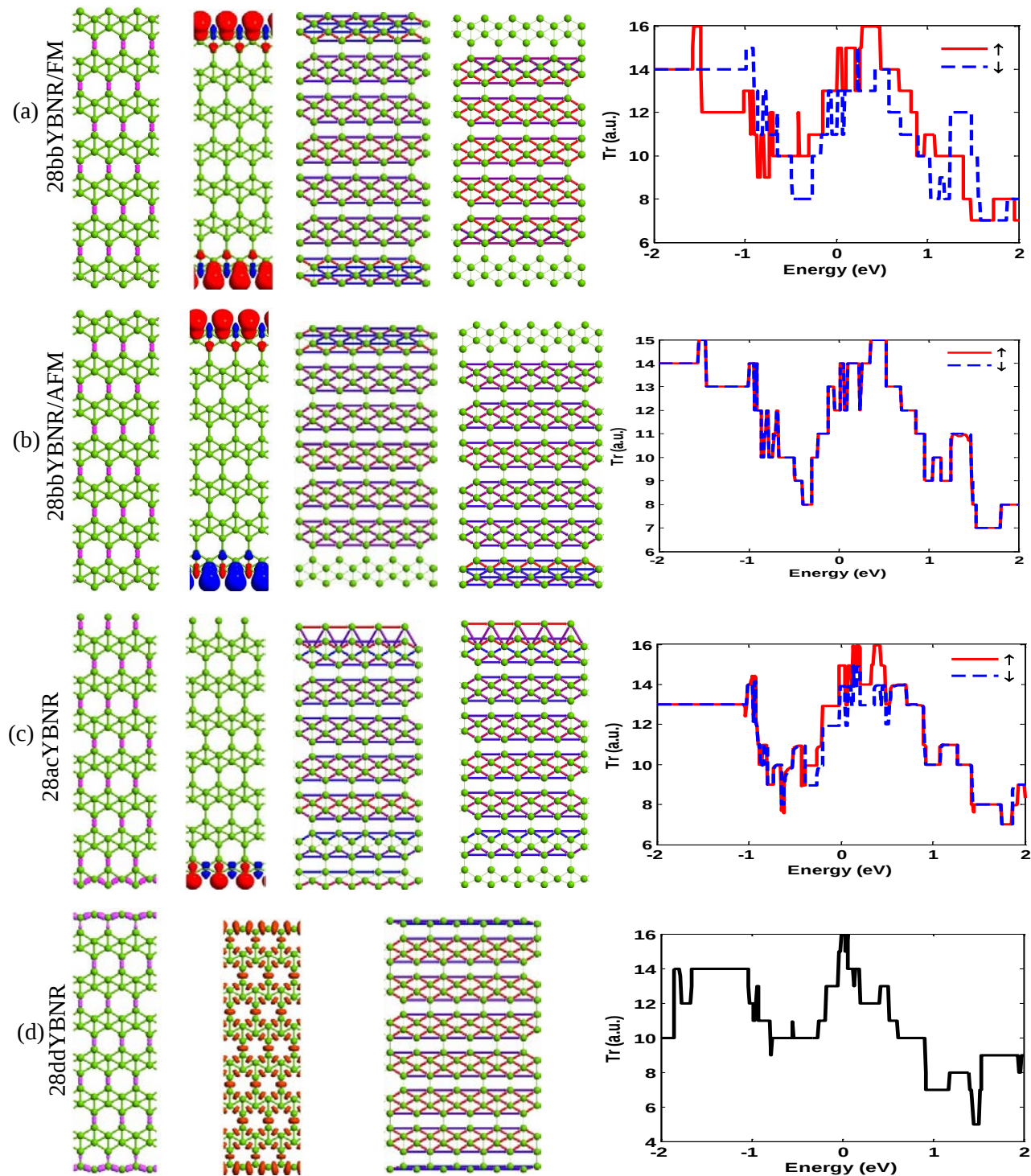


Fig. S4

Fig. S5: Ab-initio molecular dynamic, calculated by density functional tight binding (DFTB) approach for (a) 12XBNR, (b) 13XBNR, (c) 26aaYBNR and (d) 26ccYBNR after 2ps at room temperature.

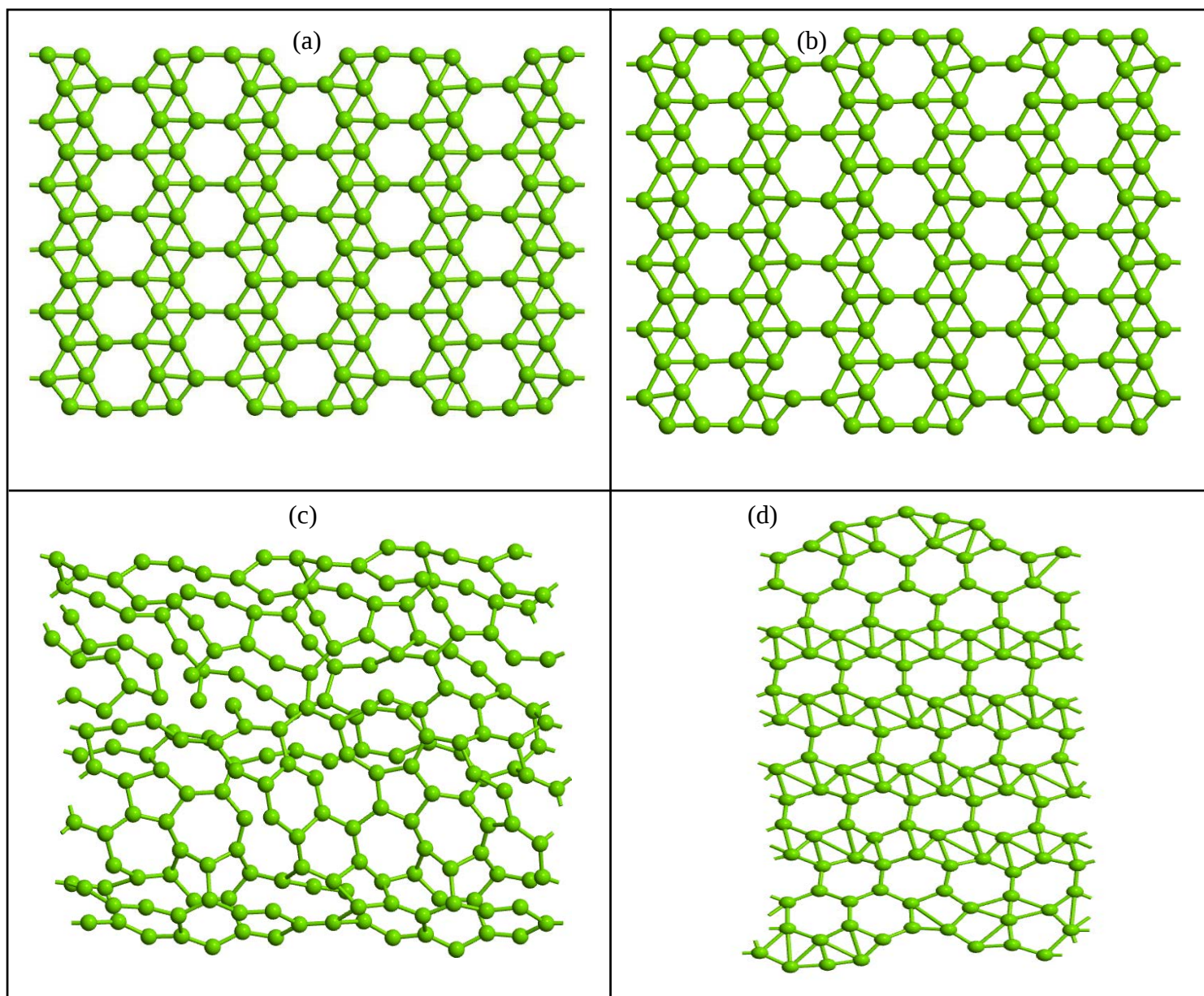


Fig. S5

Table S1: The bonding lengths of edge atoms of investigated YBNRs.

YBNR	1 st Edge							2 nd Edge						
	1-2	1-3	2-3	2-4	3-4	3-5	4-5	1-2	1-3	2-3	2-4	3-4	3-5	4-5
21ad	1.619	1.633	1.798	*	*	*	*	1.529	2.484	1.650	3.002	1.771	*	*
25ad	1.615	1.634	1.796	*	*	*	*	1.527	2.493	1.653	3.002	1.767	*	*
29ad	1.616	1.634	1.794	*	*	*	*	1.527	2.450	1.651	3.000	1.767	*	*
21bc	1.683	1.685	1.705	1.797	1.741	*	*	1.654	2.921	1.708	1.706	1.691	1.746	1.729
25bc	1.683	1.685	1.706	1.800	1.741	*	*	1.652	2.921	1.709	1.708	1.691	1.746	1.729
29bc	1.684	1.684	1.708	1.798	1.742	*	*	1.653	2.920	1.710	1.706	1.693	1.746	1.731
22aa	1.606	1.639	1.781	*	*	*	*	1.606	1.639	1.781	*	*	*	*
26aa	1.607	1.638	1.781	*	*	*	*	1.607	1.638	1.781	*	*	*	*
30aa	1.607	1.638	1.782	*	*	*	*	1.607	1.638	1.782	*	*	*	*
22bd	1.695	1.681	1.724	1.794	1.751	*	*	1.528	2.493	1.654	3.002	1.768	*	*
26bd	1.694	1.680	1.723	1.792	1.751	*	*	1.527	2.490	1.652	3.001	1.768	*	*
30bd	1.693	1.681	1.722	1.793	1.750	*	*	1.526	2.492	1.652	3.000	1.766	*	*
22cc	1.652	2.922	1.707	1.709	1.686	1.746	1.726	1.652	2.922	1.707	1.709	1.686	1.746	1.726
26cc	1.654	2.921	1.708	1.706	1.690	1.747	1.729	1.654	2.921	1.708	1.706	1.690	1.747	1.729
30cc	1.653	2.921	1.709	1.707	1.690	1.746	1.729	1.653	2.921	1.709	1.707	1.690	1.746	1.729
23ab	1.606	1.638	1.780	*	*	*	*	1.685	1.683	1.709	1.798	1.743	*	*
27ab	1.607	1.638	1.781	*	*	*	*	1.686	1.684	1.710	1.797	1.743	*	*
31ab	1.607	1.638	1.781	*	*	*	*	1.685	1.684	1.710	1.799	1.744	*	*
23cd	1.651	2.918	1.718	1.703	1.709	1.743	1.739	1.527	2.492	1.652	3.000	1.767	*	*
27cd	1.652	2.918	1.718	1.703	1.707	1.743	1.738	1.526	2.493	1.652	3.000	1.765	*	*
31cd	1.651	2.918	1.717	1.704	1.706	1.744	1.737	1.525	2.495	1.652	3.000	1.764	*	*
24bb	1.685	1.684	1.709	1.798	1.743	*	*	1.685	1.684	1.709	1.798	1.743	*	*
28bb	1.685	1.684	1.709	1.799	1.743	*	*	1.685	1.684	1.709	1.799	1.743	*	*
32bb	1.686	1.683	1.710	1.797	1.744	*	*	1.686	1.683	1.710	1.797	1.744	*	*
24ac	1.605	1.639	1.778	*	*	*	*	1.654	2.921	1.710	1.706	1.692	1.746	1.730
28ac	1.605	1.639	1.778	*	*	*	*	1.652	2.920	1.710	1.707	1.693	1.746	1.730
32ac	1.607	1.638	1.780	*	*	*	*	1.653	2.920	1.711	1.705	1.694	1.746	1.731
24dd	1.537	2.478	1.652	3.009	1.781	*	*	1.537	2.478	1.652	3.009	1.781	*	*
28dd	1.534	2.485	1.654	3.008	1.777	*	*	1.534	2.485	1.654	3.008	1.777	*	*
32dd	1.533	2.483	1.652	3.007	1.776	*	*	1.533	2.483	1.652	3.007	1.776	*	*