Supporting data

$B_3C_2N_3$ monolayer with vacancy defects decorated with lithium as a potential hydrogen storage system: A DFT study

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Table S1. Atomic coordinates of the desired structures.				
System	Atomic coordinates			
		X	Y	Z
	N	1.53781	1.07274	9.60251
	B	0.2739	1.8412	9.60251
	C	4.04781	1.12293	9.60251
	B	2.80173	1.8412	9.60251
	N	0.24006	3.32054	9.60251
	C	-0.9722	4.01998	9.60251
	N	2.83557	3.32054	9.60251
	B	1.53782	4.03187	9.60251
	N	6.55781	1.07274	9.60251
	B	5.2939	1.8412	9.60251
	C	9.06781	1.12293	9.60251
	B	7.82173	1.8412	9.60251
	N	5.26006	3.32054	9.60251
	C	4.04782	4.01998	9.60251
	N	7.85557	3.32054	9.60251
$B_3C_2N_3$	B	6.55782	4.03187	9.60251
	N	-0.9722	5.42019	9.60251
	B	-2.2361	6.18865	9.60251
	C	1.53781	5.47038	9.60251
	B	0.29173	6.18865	9.60251
	N	-2.2699	7.66799	9.60251
	C	-3.4822	8.36743	9.60251
	N	0.32557	7.66799	9.60251
	B	-0.9722	8.37931	9.60251
	N	4.04781	5.42019	9.60251
	B	2.7839	6.18865	9.60251
	C	6.55781	5.47038	9.60251
	B	5.31173	6.18865	9.60251
	N	2.75006	7.66799	9.60251
	C	1.53782	8.36743	9.60251
	N	5.34557	7.66799	9.60251
	B	4.04782	8.37931	9.60251
	N	2.861403	1.989663	17.86842
	B	0.494306	3.47317	17.4616
	C	7.645498	2.123555	18.61675
	B	5.135347	3.436327	18.76747
Li-V_C	N	0.389967	6.262219	17.87903
	C	-1.84164	7.573421	17.77377
	N	4.768634	5.944768	19.50051
	B	2.788045	7.513763	18.7348
	N	12.42911	1.989502	17.8716

	B	10.15655	3.435636	18.77558
	C	17.13123	2.134323	16.81415
	B	14.79579	3.47323	17.46375
	N	10.52647	5.941115	19.51813
	N	14.8998	6.26228	17.88199
	B	12.50333	7.512524	18.74695
	N	-1.84177	10.25114	17.68911
	B	-4.25351	11.68382	17.82868
	C	2.903502	10.33999	18.54003
	B	0.569978	11.68439	17.82413
	N	-4.28671	14.49369	17.67634
	C	-6.60716	15.8322	17.74853
	N	0.603824	14.49403	17.67527
	B	-1.84119	15.87098	17.84784
	N	7.644432	10.891	19.37973
	B	5.293021	11.85007	18.67498
	C	12.38713	10.33973	18.55119
	B	9.997094	11.85024	18.67977
	N	5.17733	14.55289	17.82545
	C	2.924428	15.83236	17.74872
	N	10.1129	14.55254	17.82593
	B	7.645163	15.86546	17.42438
	Li	7.643106	7.618425	20.95303

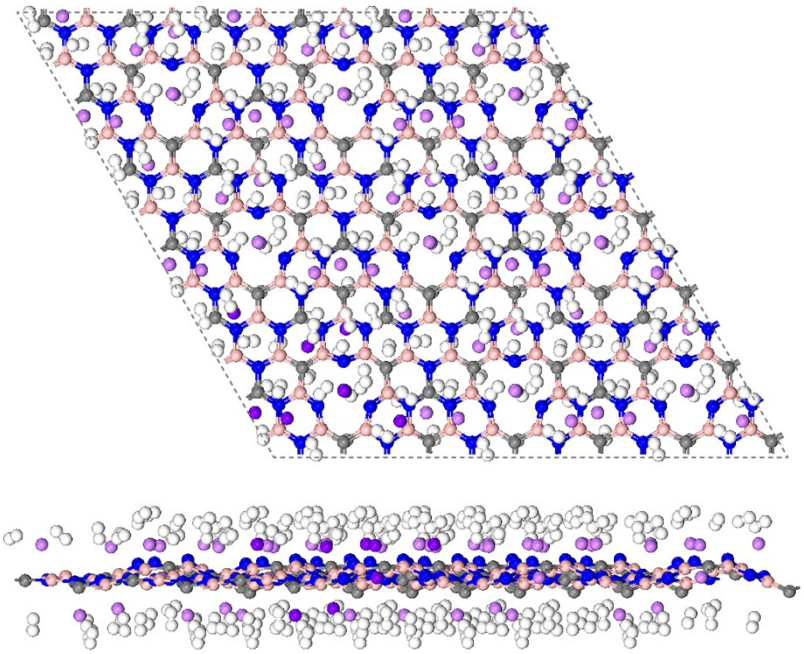

Fig. S1. Top and side view of the extended structures for H_2 molecules adsorption on V_C decorated by Li atoms.

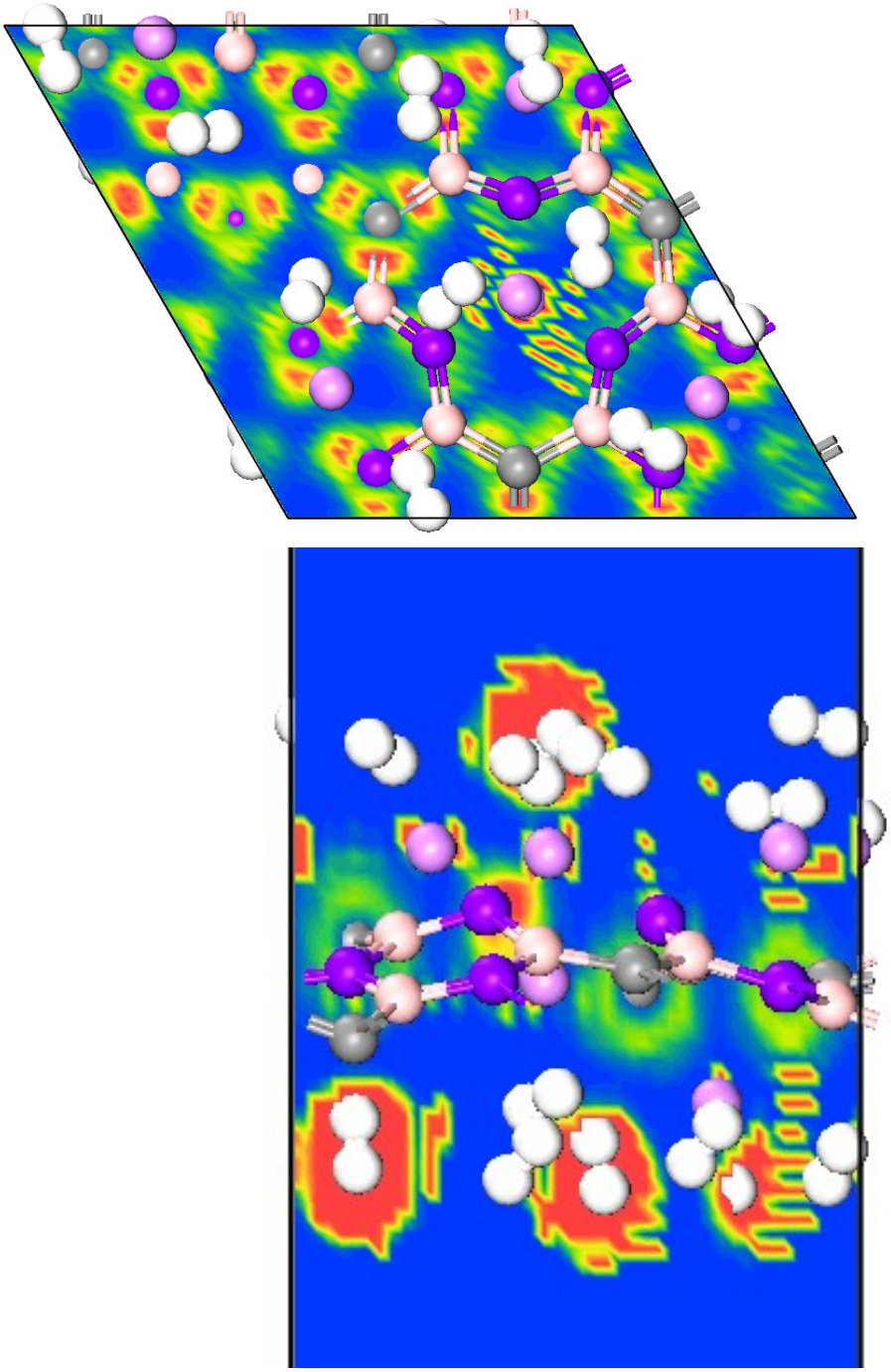

Fig. S2. Electron Localization Function (ELF) plot for the $20H_2$-8Li-V_C complex. The ELF values, which range from 0 to 1, are represented on a red-green-blue color scale.