Supplementary Information

Carbon Nitride Monolayer Nanosheets: Astrochemical Insights into the Fate of Interstellar Hydrogen

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Table 1: Energy potential minima (eV) and their corresponding sites calculated for each graphitic-like carbon nitride nanosheet, as shown in Figure 2.

2D-CN	**Site**	**Minimum potential (eV)**	**D3 correction (eV)**	z_{min} **(Å)**
C_2N_1	C	-1.038	−0.038	1.23
C_2N_1	C-C	-1.066	−0.020	1.13
C_2N_1	C-N	-0.541	−0.023	1.13
C_2N_1	N	-1.706	−0.037	1.03
C_2N_1	centre1	-0.178	−0.083	1.63
C_2N_1	centre2	-0.039	−0.044	2.83
C_2N_1	centre3	-0.296	−0.078	0.43
C_3N_1	C	-0.240	−0.064	2.42
C_3N_1	N	-0.177	−0.046	2.87
C_3N_1	C-N	-0.200	−0.053	2.71
C_3N_1	C-C	-0.243	−0.063	2.44
C_3N_1	centre1	-0.189	−0.055	2.66
C_3N_1	centre2	-0.254	−0.063	2.44
C_3N_2	C	-2.193	−0.036	1.14
C_3N_2	C-C	-2.937	−0.032	1.14
C_3N_2	C-N	-2.438	−0.026	1.04
C_3N_2	N	-3.120	−0.032	1.04
C_3N_2	NN1	-4.177	−0.039	0.04 [1]
C_3N_2	centre1	-3.831	−0.100	0.04 [1]
C_3N_2	centre2	-1.571	−0.082	0.04 [1]
C_3N_4	C	-0.075	−0.040	2.88
C_3N_4	N1	-0.554	−0.042	1.07
C_3N_4	N2	-0.072	−0.038	2.97
C_3N_4	C-N	-0.077	−0.042	2.84
C_3N_4	centre1	-0.080	−0.041	2.89
C_3N_4	centre2	-2.922	−0.041	0.00
C_3N_4	centre3	-0.075	−0.045	2.73
C_4N_3	C1	-3.048	−0.037	1.15
C_4N_3	C2	-1.202	−0.038	1.18
C_4N_3	N	-2.993	−0.045	1.05
C_4N_3	C-N	-1.549	−0.025	1.09
C_4N_3	C-C	-2.178	−0.018	1.10
C_4N_3	centre1	-0.434	−0.052	0.90
C_4N_3	centre2	-5.374	−0.052	0.00
C_6N_6	C	-0.687	−0.036	1.19
C_6N_6	C-C	-0.827	−0.022	1.09
C_6N_6	C-N	-0.241	−0.025	1.09
C_6N_6	N	-1.566	−0.034	1.09
C_6N_6	NN1	-0.532	−0.041	0.69
C_6N_6	centre1	-0.250	−0.075	0.59
C_6N_6	centre2	-0.022	−0.033	3.09
C_6N_8	C	-0.222	−0.038	1.21

[1]The plots given in Figure 2 of the main paper clearly show that the true minimum is at 0 Å, but we faced numerical instabilities when trying to converge this point. As the Figure shows, this has a negligible impact as we are sufficiently close to the minimum.

2D-CN	**Site**	**Minimum potential (eV)**	**D3 correction (eV)**	z_{min} **(Å)**
C_6N_8	C-N1	-0.064	−0.043	2.71
C_6N_8	C-N2	-0.087	−0.043	2.81
C_6N_8	N	-0.090	−0.042	2.91
C_6N_8	centre1	-0.051	−0.082	1.11
C_6N_8	centre2	-0.078	−0.043	2.81
C_6N_8	centre3	-0.047	−0.042	2.71
C_9N_4	C	-1.062	−0.043	1.19
C_9N_4	C-C	-0.994	−0.019	1.19
C_9N_4	C-N	-0.223	−0.056	2.59
C_9N_4	N	-0.178	−0.046	2.89
C_9N_4	centre1	-0.133	−0.078	0.59
C_9N_4	centre2	-0.635	−0.082	1.79
C_9N_4	centre3	-0.191	−0.055	2.59
C_9N_7	C	-2.067	−0.072	1.20
C_9N_7	C-C	-2.401	−0.023	1.10
C_9N_7	C-N	-1.053	−0.073	1.10
C_9N_7	N	-0.973	−0.074	1.10
C_9N_7	centre1	-1.001	−0.029	1.10
C_9N_7	centre2	-0.710	−0.023	1.00
C_9N_7	centre3	-0.987	−0.057	1.00
C_9N_7	centre4	-0.472	−0.049	0.00

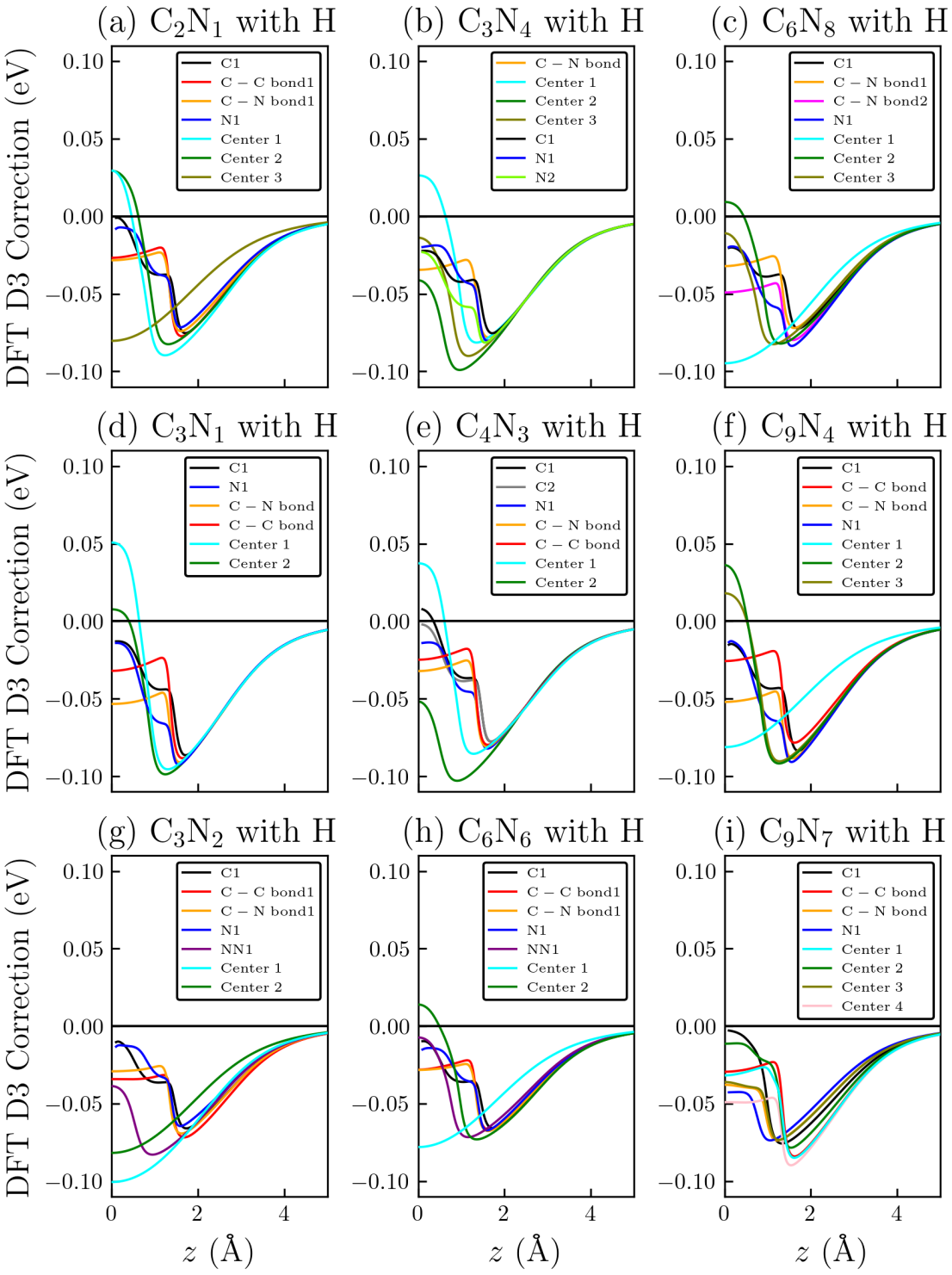

Figure 1: DFT-D3 dispersion-correction as a function of distance from the sheet for a hydrogen atom at specific sheet position.