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Supporting Information

N_2 reduction on uranium-doped C_2N/C_3N_4 monolayers: A DFT computational study

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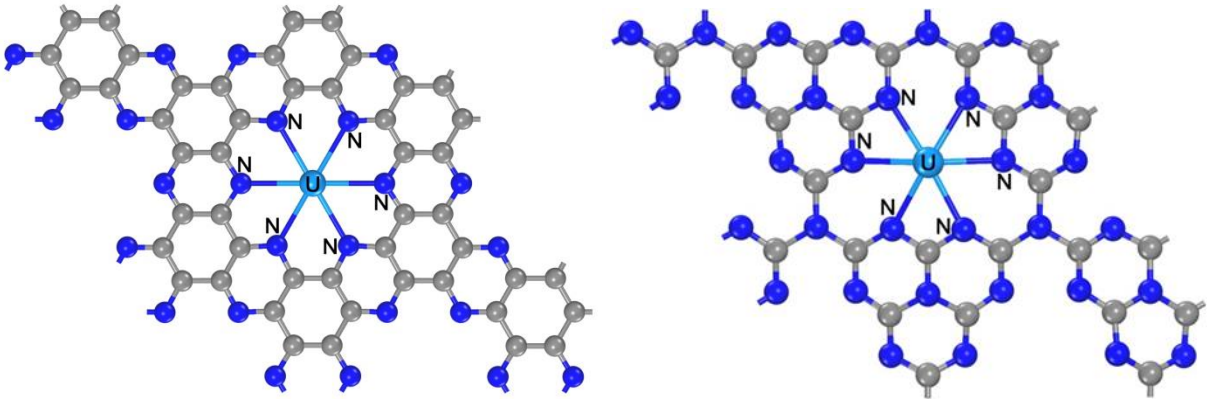
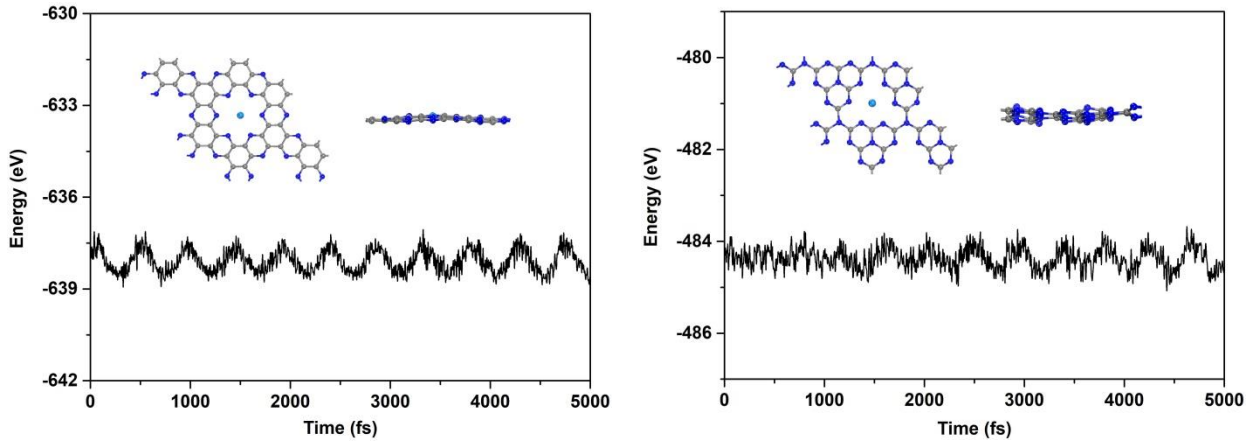


U-N average bond length: 2.680 Å (a)

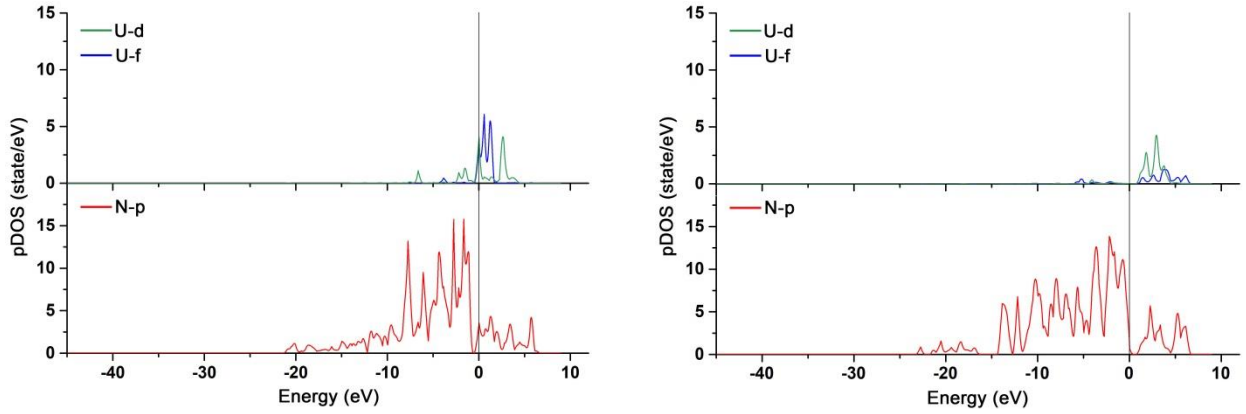
U-N average bond length: 2.432 Å (b)

Fig. S1 Top and side views of optimized structures of (a) U-C_2N and (b) U-C_3N_4 with full N-U bonds and U-N average bond lengths. The colors of the spheres have the same meaning of atoms in **Fig. 1**.



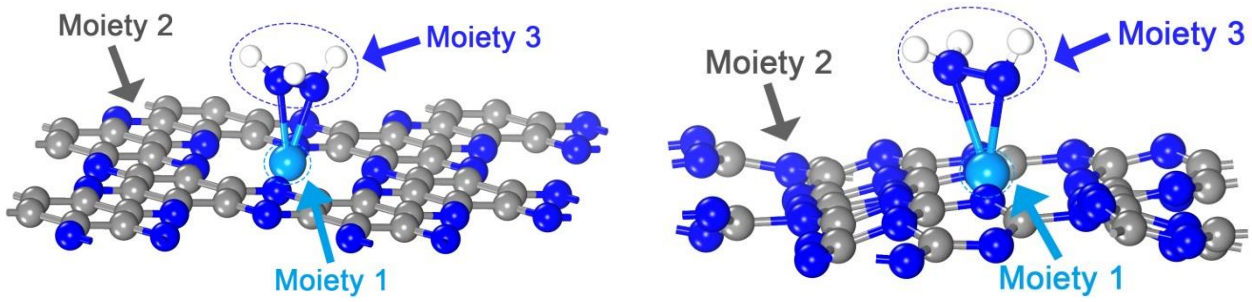
(a) (b)

Fig. S2 Variations of energy against time for AIMD simulations of (a) U-C_2N and (b) U-C_3N_4. The simulation is run at 300 K for 5 ps with a time step of 1 fs.



(a) (b)

Fig. S3 The pDOS of (a) U-C_2N and (b) U-C_3N_4. The Fermi level is set to 0 eV.



(a) (b)

Fig. S4 The defined three moieties in *N_xH_y absorbed on (a) U-C_2N and (b) U-C_3N_4.

Table S1 Variation of Bader charge of the three moieties in the U-C_2N model.

Reaction step	Moiety 1	Moiety 2	Moiety 3
0	-0.06	-0.40	0.46
1	-0.09	-0.19	0.29
2	-0.04	0.11	-0.06
3	0.05	0.26	-0.31
4	-0.11	-0.42	0.53
5	0.11	0.33	-0.44
6	0.09	0.48	-0.57

Table S2 Variation of Bader charge of the three moieties in the U-C_3N_4 model.

Reaction step	Moiety 1	Moiety 2	Moiety 3
0	-0.24	-0.27	0.50
1	-0.10	-0.11	0.21
2	-0.22	-0.55	0.78
3	0.23	0.80	-1.03
4	-0.17	-0.35	0.52
5	0.18	0.27	-0.45
6	0.09	0.54	-0.63