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Supporting Information

Al-embedded C_2N: DFT Study on a Promising Catalyst for CO Oxidation

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Table S1. The computed energies (E, a.u.) of various species by considering different spin-state in the present work.

	S=1/2	S=3/2	S=0	S=1
Al	-242.368235	-242.229243	-	-
Al-C_2N	-2278.319881	-2278.312415	-	-
O_2	-	-	-150.253684	-150.316263
O_2/C_2N	-	-	-2186.088193	-2186.147104
O_2/Al-C_2N	-2428.73254	-2428.712275	-	-

O_2 + CO/Al-C_2N	-2542.209548	-2542.022506		

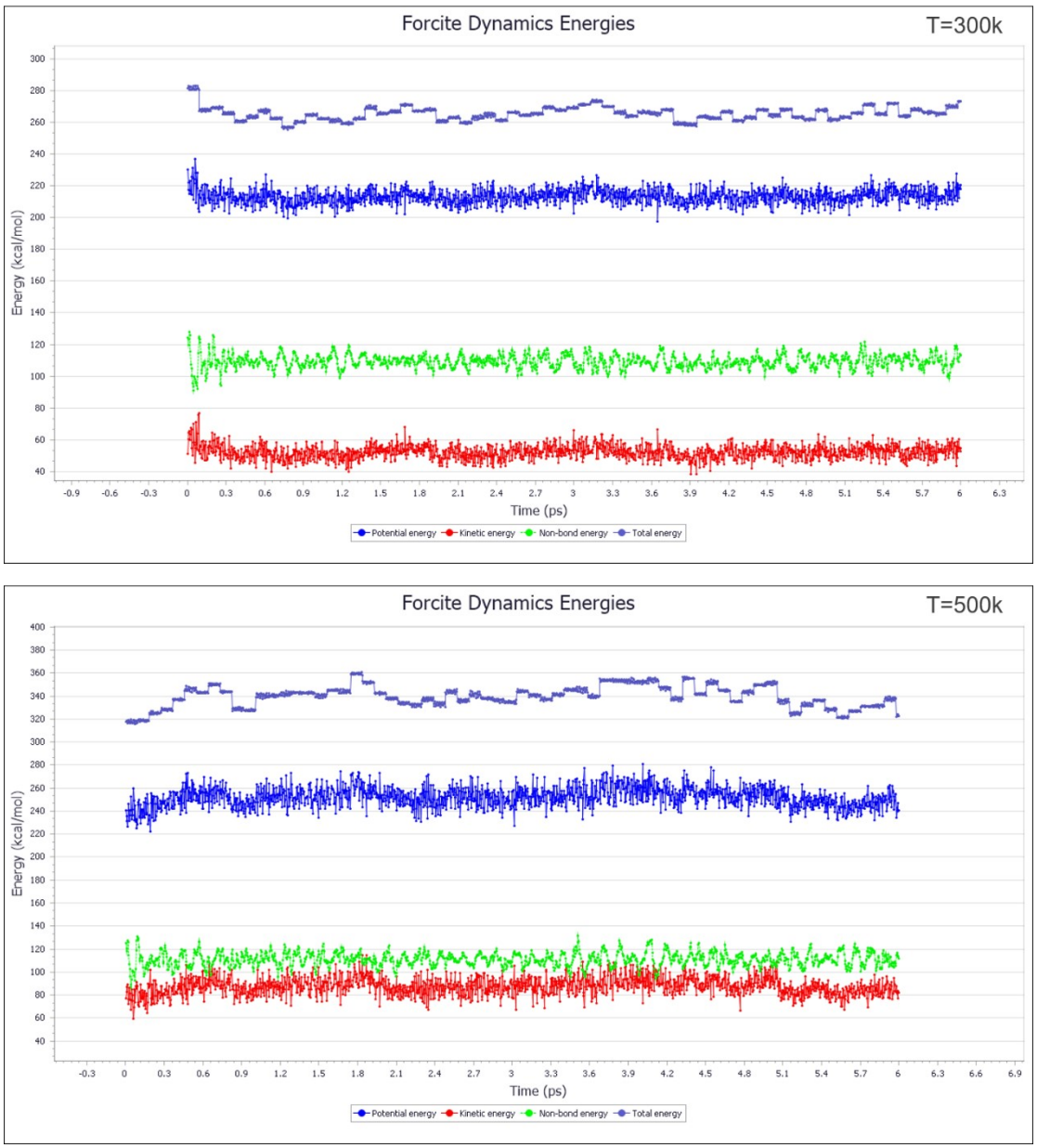

Fig. S1. Molecular dynamics simulations of Al-C_2N at 300 and 500 K, respectively.

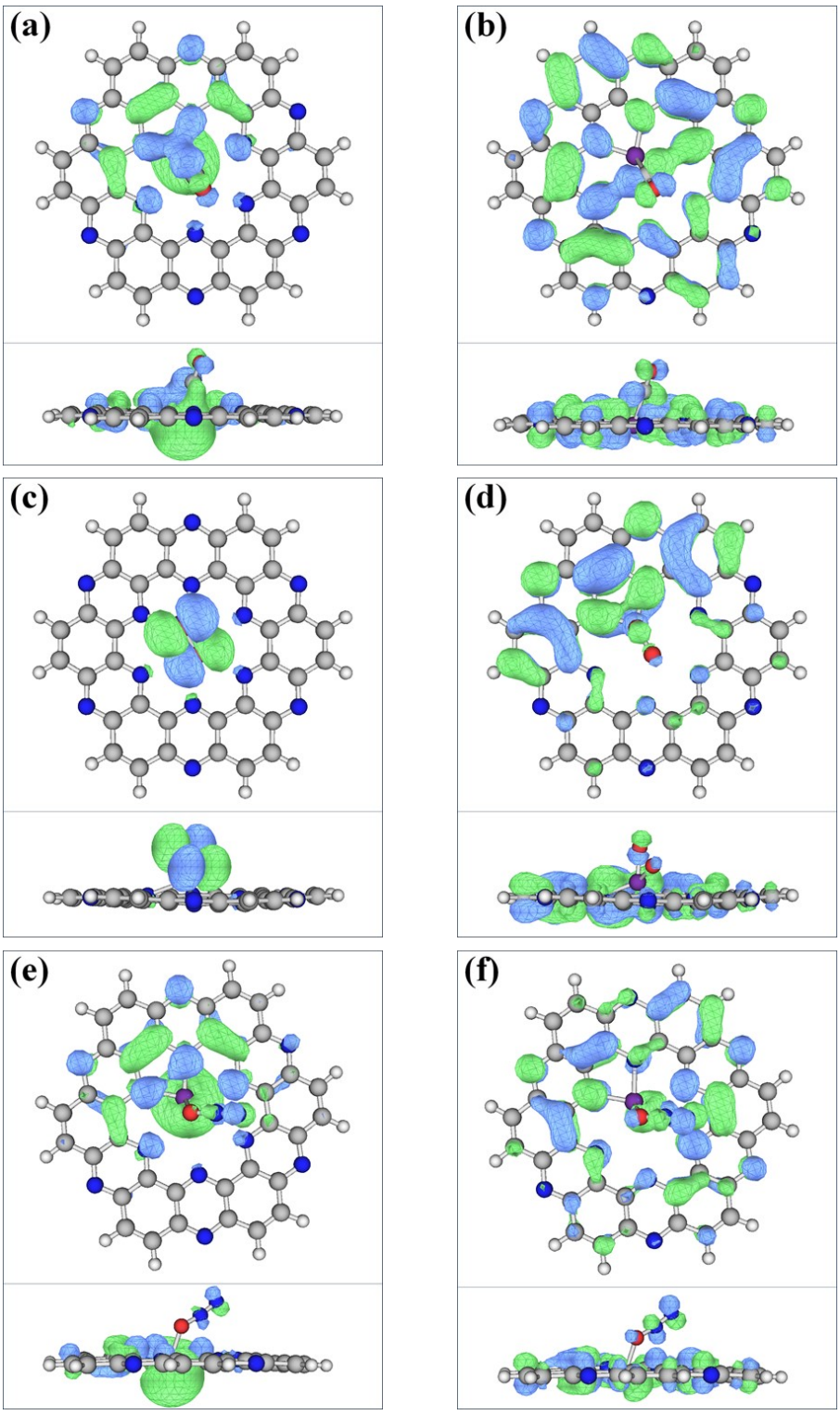

Fig. S2. HOMO (a, c, e) and LUMO (b, d, f) orbitals of the Al-C_2N surface after gas adsorption.

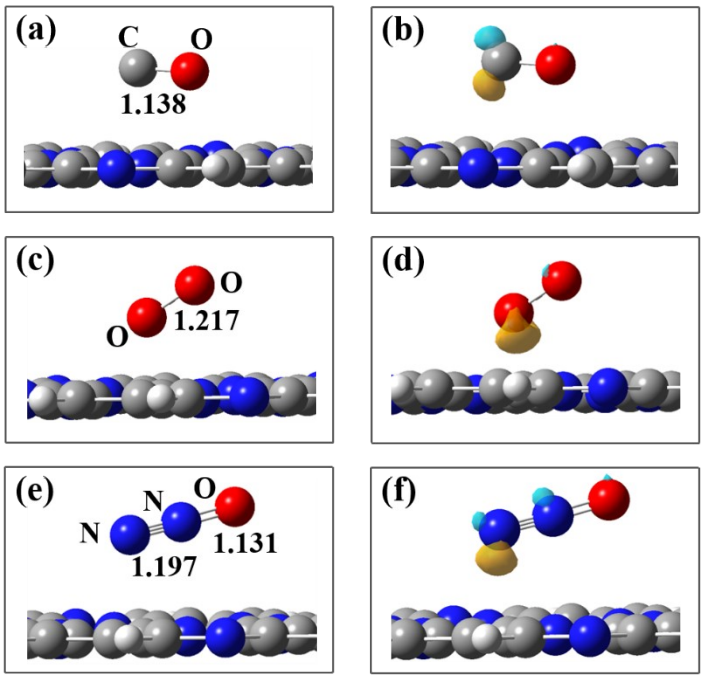

Fig. S3. The local configurations and relevant structural parameters for CO, O_2, and N_2O adsorption on the C_2N monolayer are shown in (a), (c), and (e), respectively. The EDD plots (in 0.003 au) for CO, O_2, and N_2O on the C_2N monolayer are shown in (b), (d), and (f), respectively. Blue and yellow regions represent the charge accumulation and depletion, respectively. All bond distances are given in Å.