Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

for

Atomic Insights into the Interaction of N_2, CO_2, NH_3, NO, and NO_2 Gas Molecules with the Zn_2(V, Nb, Ta)N_3 Ternary Nitride Monolayers

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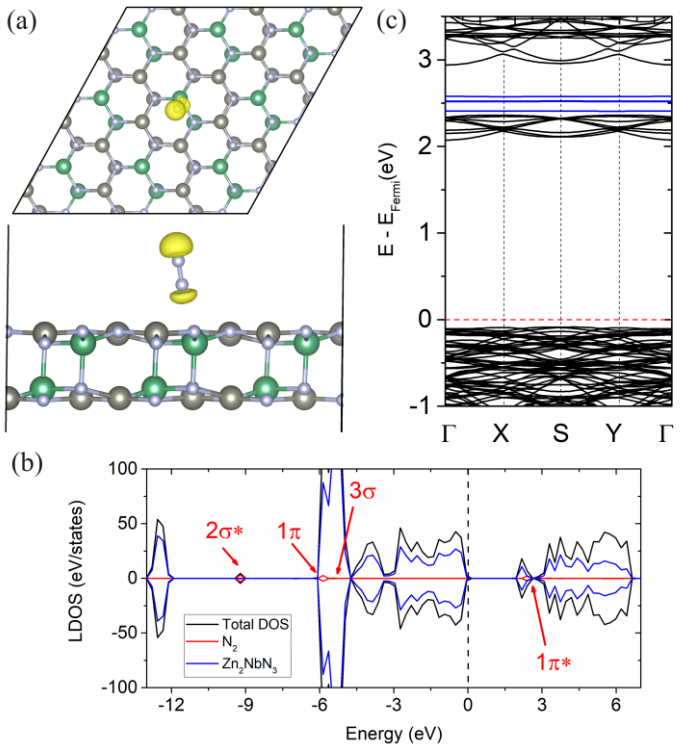

Figure S1. (a) The top and side views of the lowest-energy configuration combined with the ELF plots (the isosurface level of 0.75 is adopted here) for the Zn_2NbN_3 monolayer adsorbed with the N_2 molecule. (b) The total DOS (black line) and LDOS (red and blue lines) of the Zn_2NbN_3 monolayer adsorbed with the N_2 molecule. The vertical black dashed line shows the Fermi level. (c) The band structure of the Zn_2NbN_3 monolayer adsorbed with the N_2 molecule. The horizontal red dashed line shows the Fermi level.

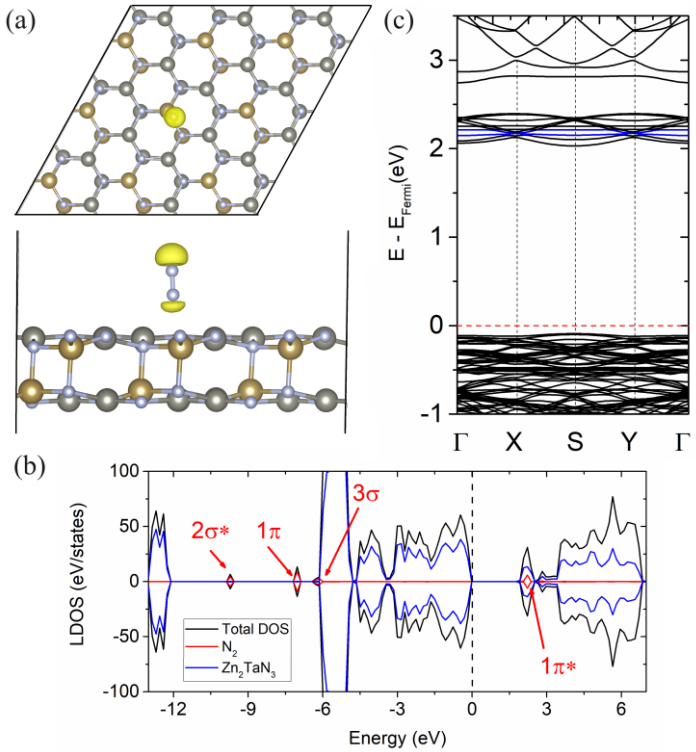

Figure S2. (a) The top and side views of the lowest-energy configuration combined with the ELF plots (the isosurface level of 0.75 is adopted here) for the Zn_2TaN_3 monolayer adsorbed with the N_2 molecule. (b) The total DOS (black line) and LDOS (red and blue lines) of the Zn_2TaN_3 monolayer adsorbed with the N_2 molecule. The vertical black dashed line shows the Fermi level. (c) The band structure of the Zn_2TaN_3 monolayer adsorbed with the N_2 molecule. The horizontal red dashed line shows the Fermi level.

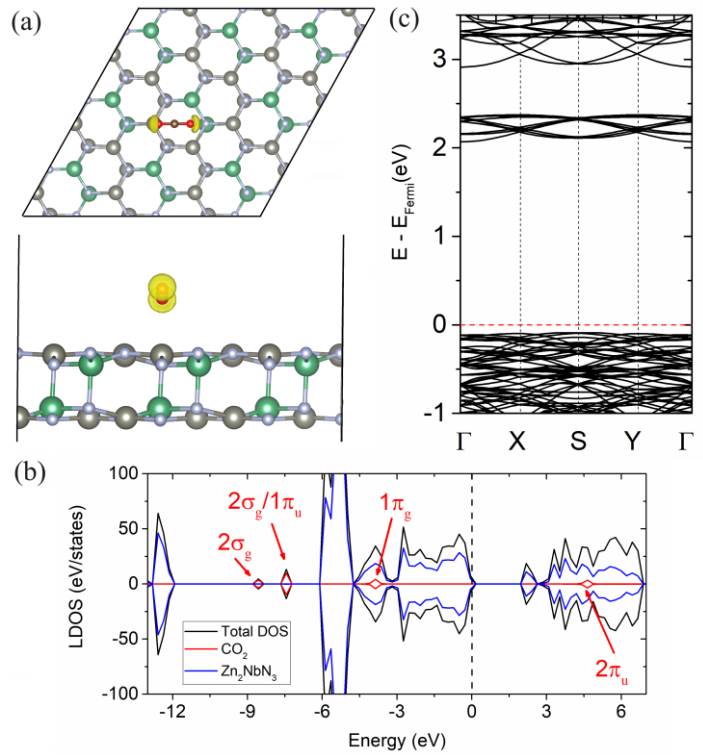

Figure S3. (a) The top and side views of the lowest-energy configuration combined with the ELF plots (the isosurface level of 0.75 is adopted here) for the Zn_2NbN_3 monolayer adsorbed with the CO_2 molecule. (b) The total DOS (black line) and LDOS (red and blue lines) of the Zn_2NbN_3 monolayer adsorbed with the CO_2 molecule. The vertical black dashed line shows the Fermi level. (c) The band structure of the Zn_2NbN_3 monolayer adsorbed with the CO_2 molecule. The horizontal red dashed line shows the Fermi level.

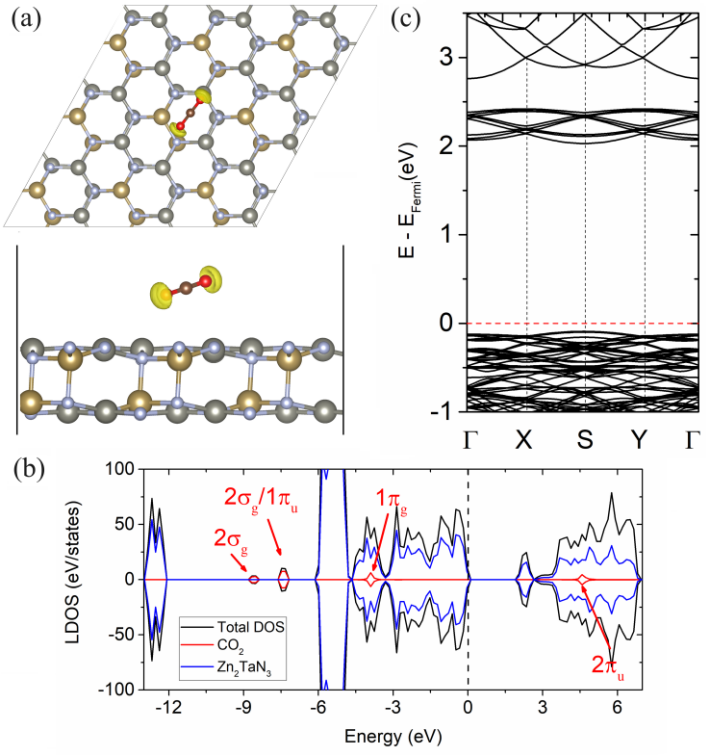

Figure S4. (a) The top and side views of the lowest-energy configuration combined with the ELF plots (the isosurface level of 0.75 is adopted here) for the Zn_2TaN_3 monolayer adsorbed with the CO_2 molecule. (b) The total DOS (black line) and LDOS (red and blue lines) of the Zn_2TaN_3 monolayer adsorbed with the CO_2 molecule. The vertical black dashed line shows the Fermi level. (c) The band structure of the Zn_2TaN_3 monolayer adsorbed with the CO_2 molecule. The horizontal red dashed line shows the Fermi level.

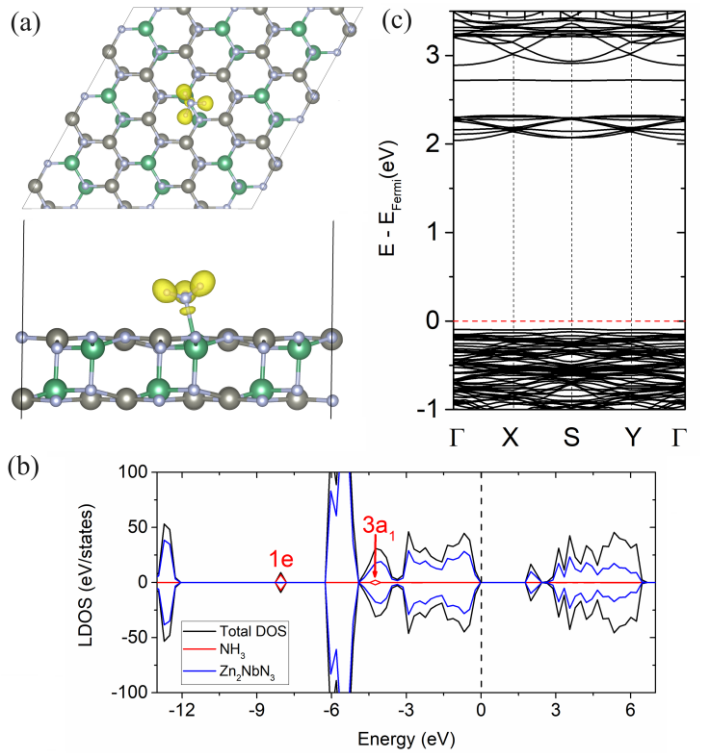

Figure S5. (a) The top and side views of the lowest-energy configuration combined with the ELF plots (the isosurface level of 0.75 is adopted here) for the Zn_2NbN_3 monolayer adsorbed with the NH_3 molecule. (b) The total DOS (black line) and LDOS (red and blue lines) of the Zn_2NbN_3 monolayer adsorbed with the NH_3 molecule. The vertical black dashed line shows the Fermi level. (c) The band structure of the Zn_2NbN_3 monolayer adsorbed with the NH_3 molecule. The horizontal red dashed line shows the Fermi level.

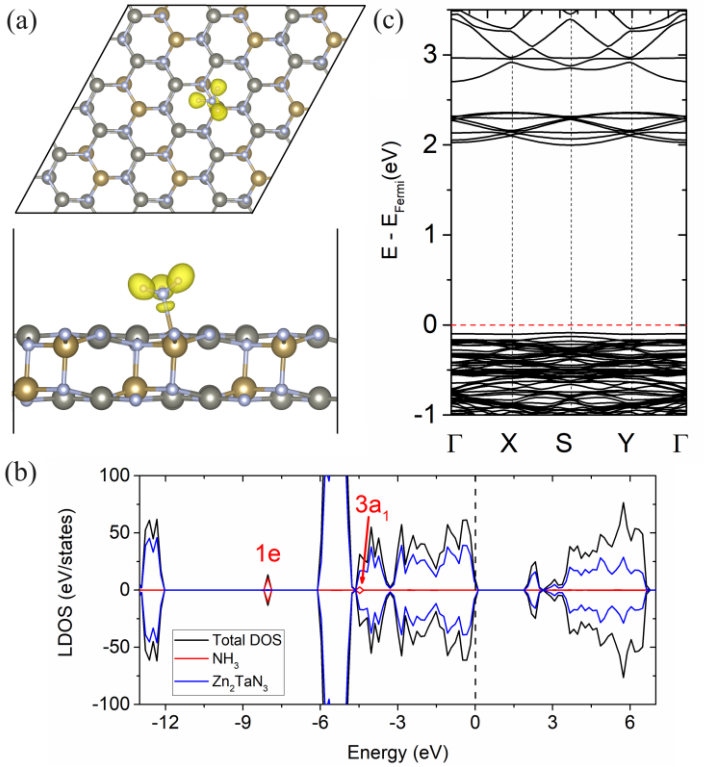

Figure S6. (a) The top and side views of the lowest-energy configuration combined with the ELF plots (the isosurface level of 0.75 is adopted here) for the Zn_2TaN_3 monolayer adsorbed with the NH_3 molecule. (b) The total DOS (black line) and LDOS (red and blue lines) of the Zn_2TaN_3 monolayer adsorbed with the NH_3 molecule. The vertical black dashed line shows the Fermi level. (c) The band structure of the Zn_2TaN_3 monolayer adsorbed with the NH_3 molecule. The horizontal red dashed line shows the Fermi level.

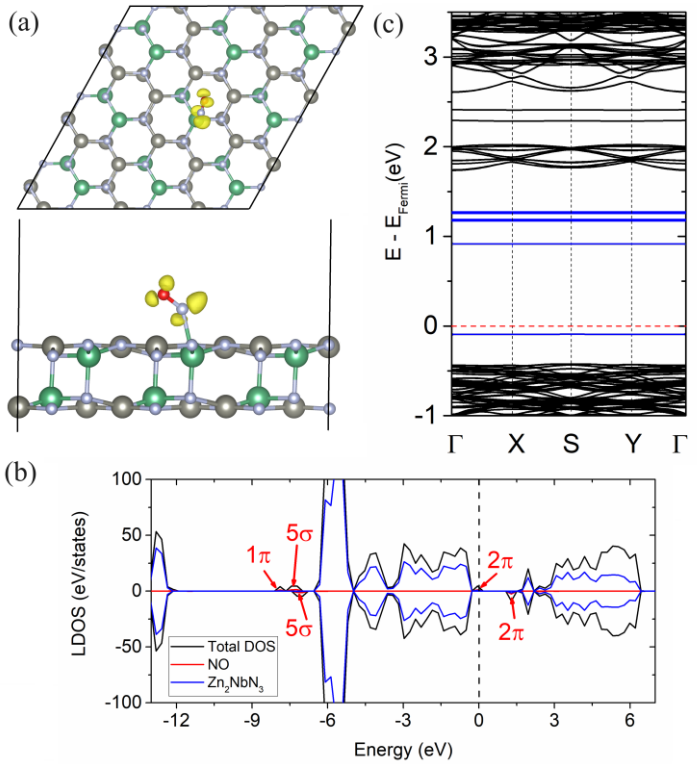

Figure S7. (a) The top and side views of the lowest-energy configuration combined with the ELF plots (the isosurface level of 0.75 is adopted here) for the Zn_2NbN_3 monolayer adsorbed with the NO molecule. (b) The total DOS (black line) and LDOS (red and blue lines) of the Zn_2NbN_3 monolayer adsorbed with the NO molecule. The vertical black dashed line shows the Fermi level. (c) The band structure of the Zn_2NbN_3 monolayer adsorbed with the NO molecule. The horizontal red dashed line shows the Fermi level.

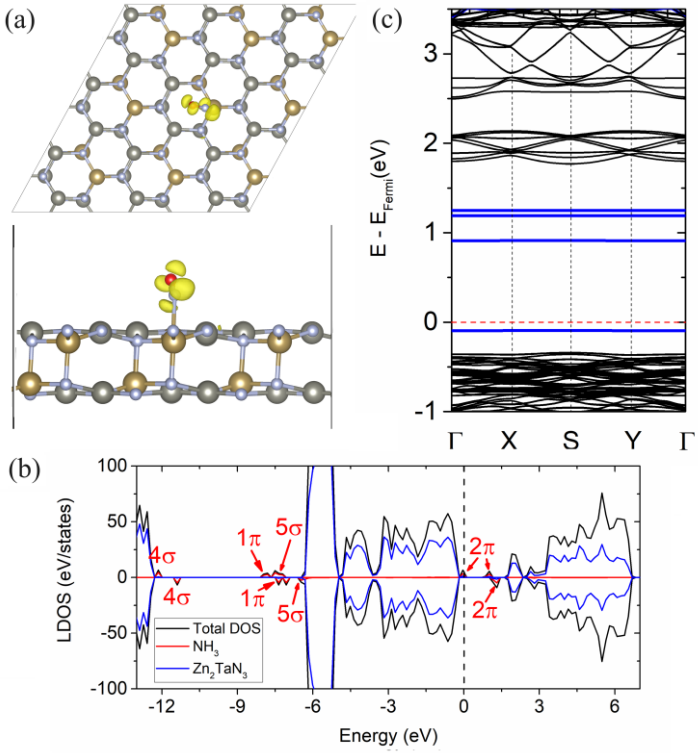

Figure S8. (a) The top and side views of the lowest-energy configuration combined with the ELF plots (the isosurface level of 0.75 is adopted here) for the Zn_2TaN_3 monolayer adsorbed with the NO molecule. (b) The total DOS (black line) and LDOS (red and blue lines) of the Zn_2TaN_3 monolayer adsorbed with the NO molecule. The vertical black dashed line shows the Fermi level. (c) The band structure of the Zn_2TaN_3 monolayer adsorbed with the NO molecule. The horizontal red dashed line shows the Fermi level.

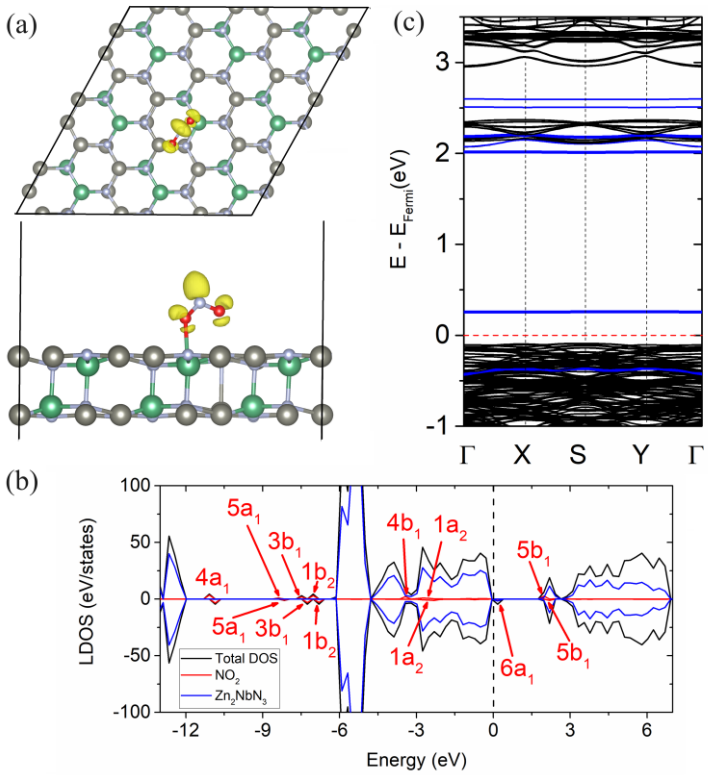

Figure S9. (a) The top and side views of the lowest-energy configuration combined with the ELF plots (the isosurface level of 0.75 is adopted here) for the Zn_2NbN_3 monolayer adsorbed with the NO_2 molecule. (b) The total DOS (black line) and LDOS (red and blue lines) of the Zn_2NbN_3 monolayer adsorbed with the NO_2 molecule. The vertical black dashed line shows the Fermi level. (c) The band structure of the Zn_2NbN_3 monolayer adsorbed with the NO_2 molecule. The horizontal red dashed line shows the Fermi level.

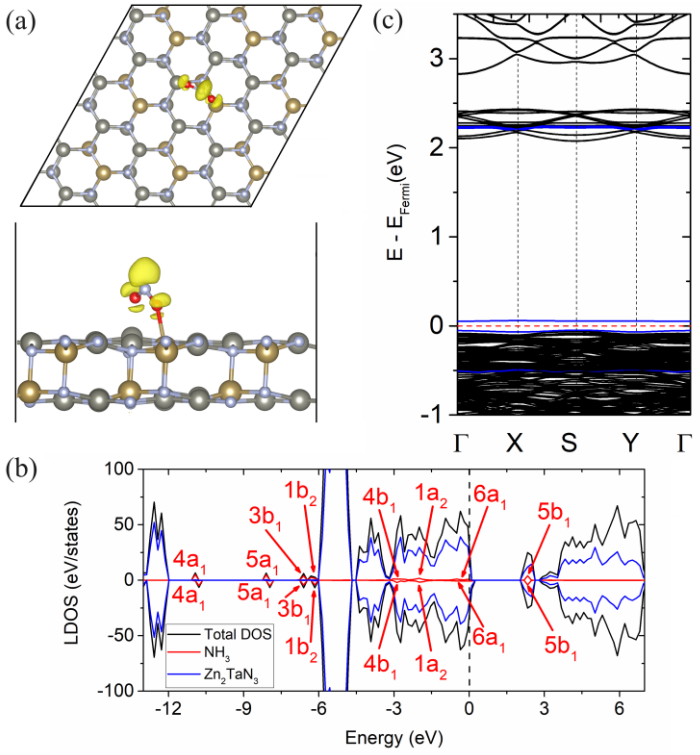

Figure S10. (a) The top and side views of the lowest-energy configuration combined with the ELF plots (the isosurface level of 0.75 is adopted here) for the Zn_2TaN_3 monolayer adsorbed with the NO_2 molecule. (b) The total DOS (black line) and LDOS (red and blue lines) of the Zn_2TaN_3 monolayer adsorbed with the NO_2 molecule. The vertical black dashed line shows the Fermi level. (c) The band structure of the Zn_2TaN_3 monolayer adsorbed with the NO_2 molecule. The horizontal red dashed line shows the Fermi level.

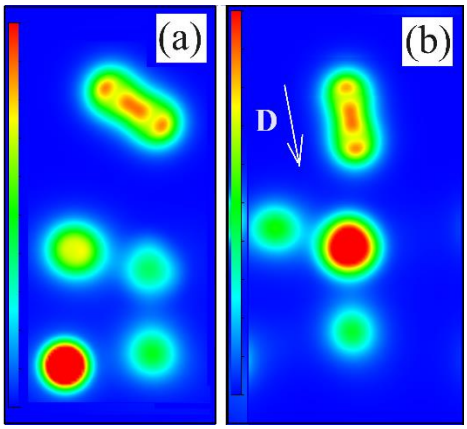

Figure S11. The ELF for the N_2 on Zn_2VN_3 (a) and Zn_2NbN_3 or Zn_2TaN_3 (b) monolayers. D denotes dipole moment.