Supplementary Information

Control of $C_3N_4$ and $C_4N_3$ carbon nitride nanosheets’ electronic and magnetic properties through embedded atoms

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The optimized structures of Li, Na, K, Be, Mg, Ca, and Al substitutionally adsorbed on $C_3N_4$ and $C_3N_4$ nanosheets, are shown in Fig. S1. The embedding of Li, Na, and K atoms, due to the stronger interaction between atoms and $C_3N_4$ and $C_3N_4$, yields a significant distortion and local deformation, where reconstructions also occur.

The DOS and PDOS of Li, Na, K, Be, Mg, Ca and Al atoms embedded into holey site of $C_3N_4$ and $C_3N_4$ nanosheets are shown in Fig. S2.

Here, we investigate the structural, electronic and magnetic properties of Sc, Ti, V, Cr,
Mn, Fe, Co, Ni, and Zn atoms embedded into holey site of $C_3N_4$ and $C_3N_4$ nanosheets. The optimized structures are shown in Fig. S3.

In order to better identify and investigate the effects of the embedding of atoms on $C_3N_4$ and $C_3N_4$ nanosheets, we simulated their STM images (Fig. S4). We can see that the C and N atoms appear as white spots; however, the region around O, P, Li, and Fe atoms corresponds to the brighter spot. With a bias of +2 V, the structures of embedded $C_3N_4$ and $C_3N_4$ nanosheets are easier to identify through their STM images.
Figure S2: DOS and PDOS of Li, Na, K, Be, Mg, Ca, and Al atoms embedded into holey site of (a) \(C_3N_4\) and (b) \(C_3N_4\) nanosheets. The zero of energy is set at \(E_F\) as shown by the dashed green line.
Figure S3: Optimized structures of Sc, Ti, V, Cr, Mn, Fe, Co, Ni and Zn atoms embedded into holey site of (a) $C_3N_4$ and (b) $C_3N_4$ nanosheets.

Figure S4: Simulated scanning tunneling microscopy (STM) images of O, P, Li and Fe Sc, Ti, V, Cr, Mn, Fe, Co, Ni, and Zn atoms embedded into holey site of (a) $C_3N_4$ and (b) $C_4N_3$ nanosheets. Simulated STM images are overlayd with the its structures.
Figure S5: DOS and PDOS of Sc, Ti, V, Cr, Mn, Fe, Co, Ni and Zn atoms embedded into holey site of $C_4N_3$ nanosheet. The zero of energy is set at $E_F$ as shown by the dashed green line.