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

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 substutionally 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,

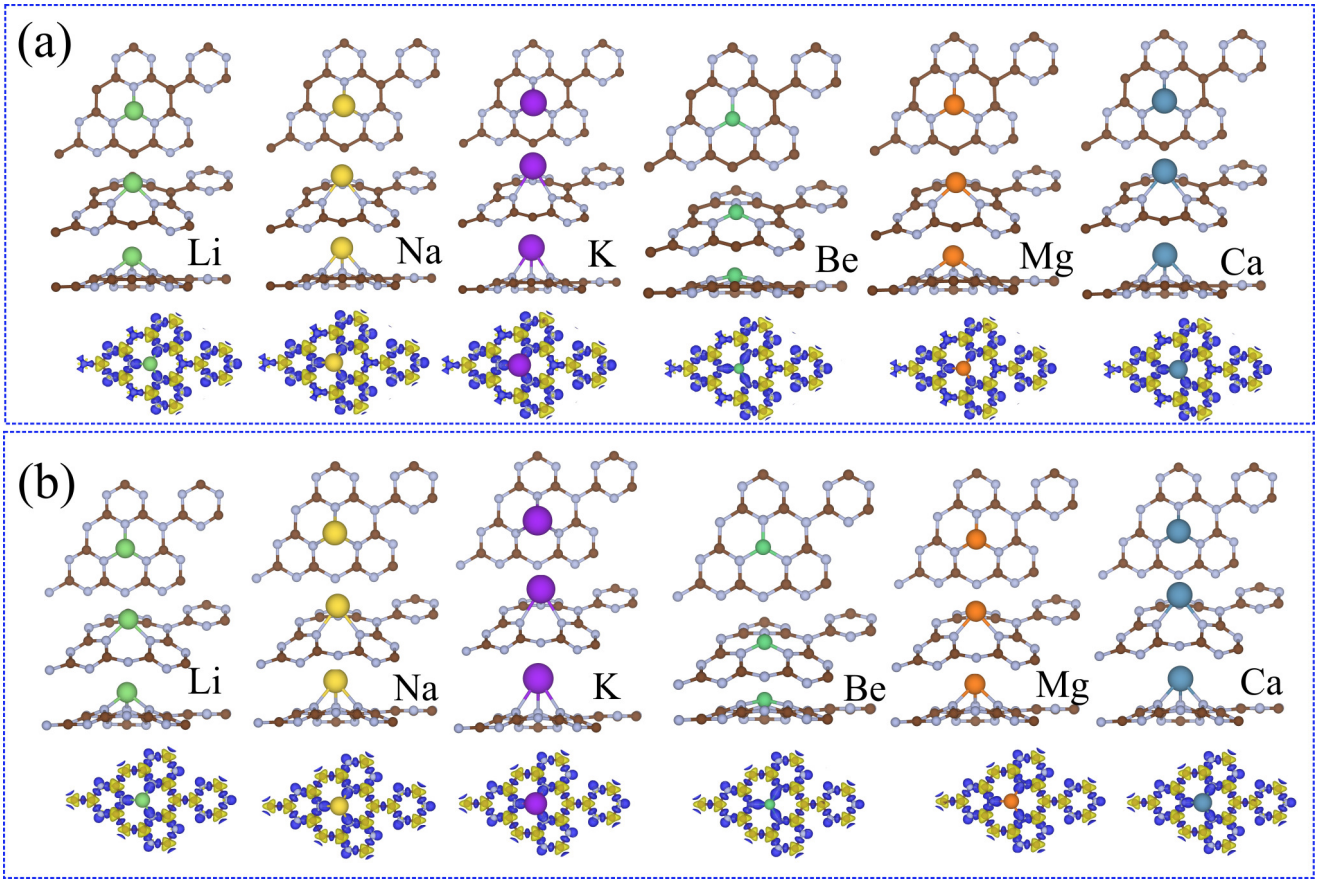

Figure S1: Optimized structures of substitutional adsorption of Li, Na, K, Be, Mg, Ca, and Al on (a) C_3N_4 and (b) C_3N_4 nanosheets. Difference charge densities are shown where the blue and yellow regions represent charge accumulation and depletion, respectively.

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.

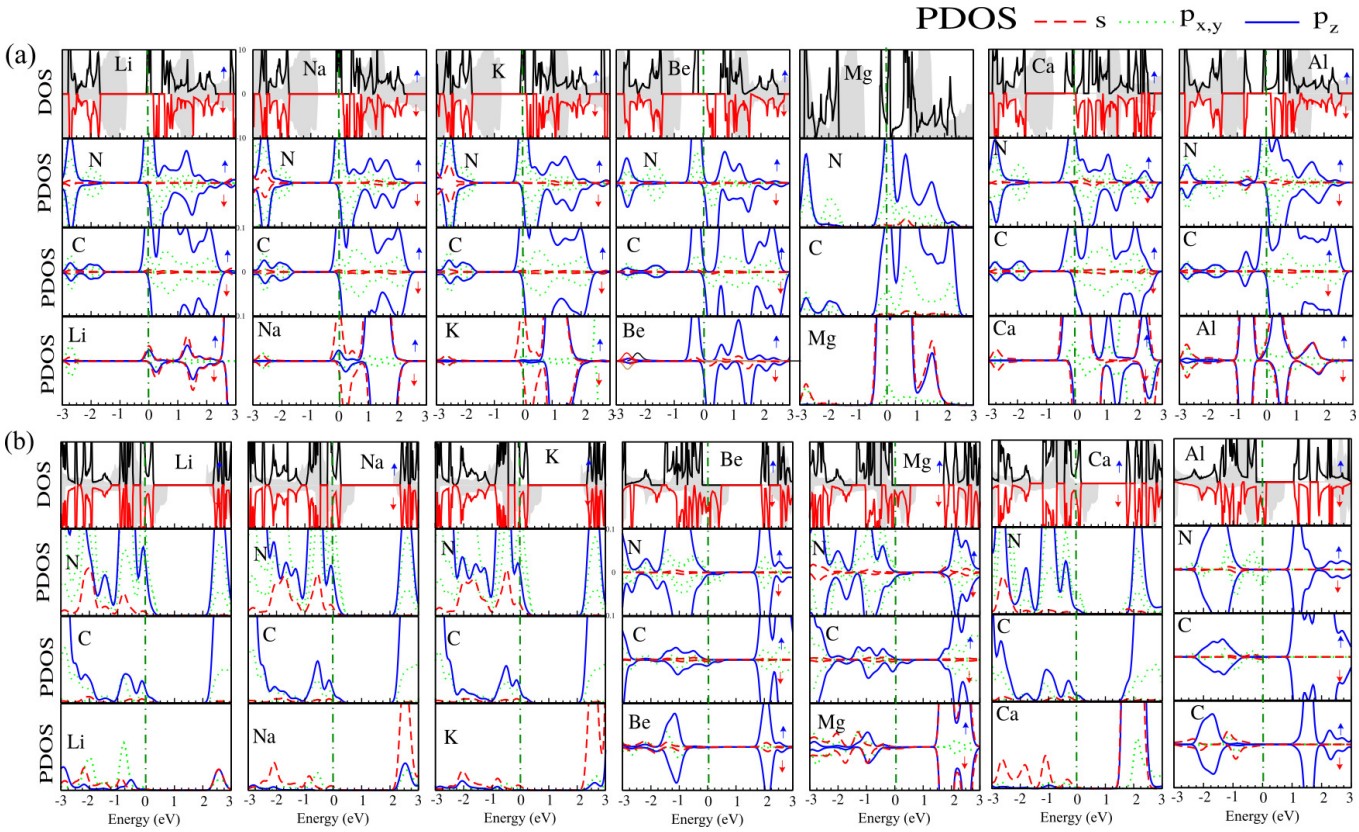

Figure S2: DOS and PDOS of Li, Na, K, Be, Mg, Ca, and Al atoms embedded into holey site of (a) C_3N_4 and (b) C_3N_4 nanosheets. The zero of energy is set at E_F as shown by the dashed green line.

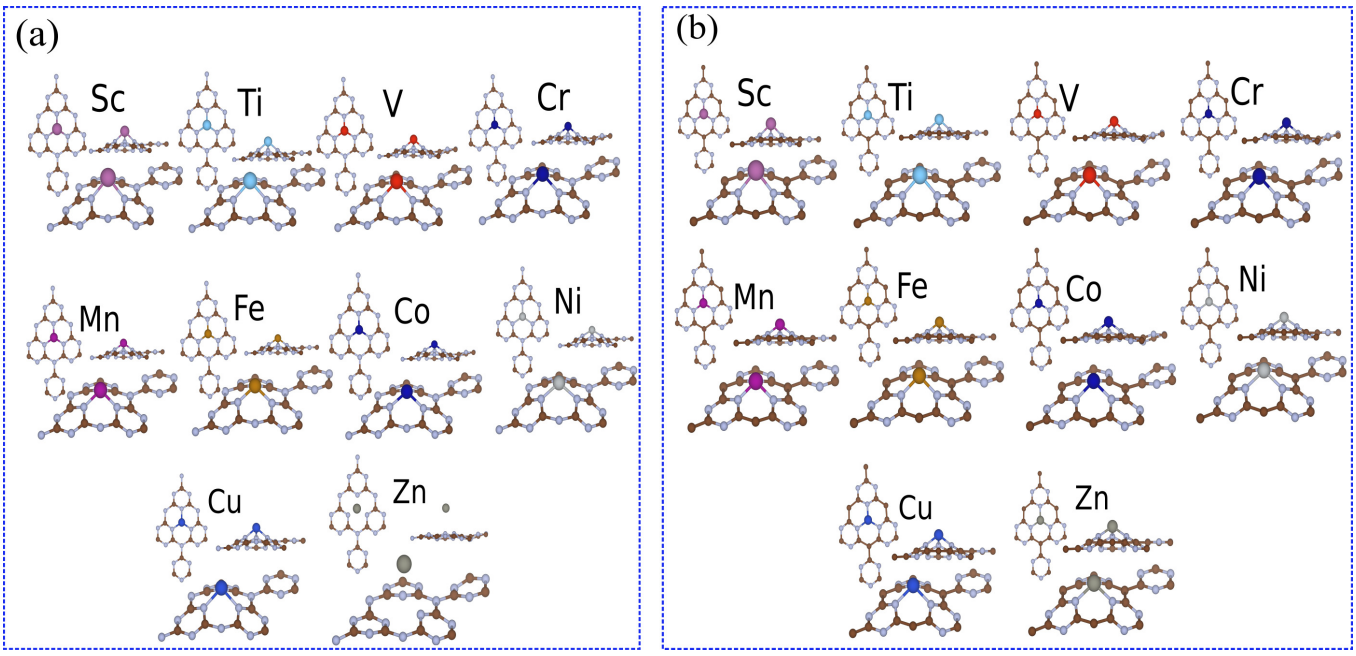

Figure S3: Optimized structures of Sc, Ti, V, Cr, Mn, Fe, Co, Ni and Zn atoms embedded into holey site of (a) C_3N_4 and (b) C_3N_4 nanosheets.

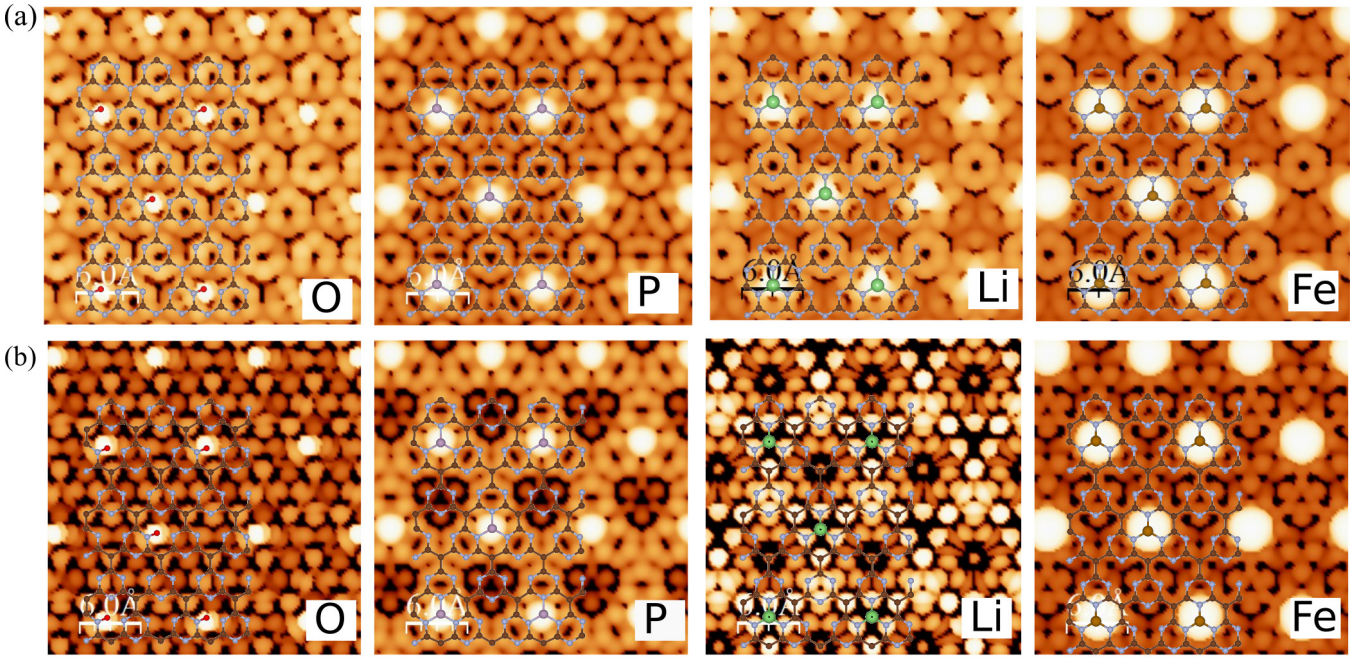

Figure S4: Simulated scanning tunneling microscopy (STM) images of O, P, Li and Fe Sc, Ti, V, Cr, Mn, Fe, Co, Ni, and Zn atoms embedded into holey site of (a) C_3N_4 and (b) C_4N_3 nanosheets. Simulated STM images are overlayd with the its structures.

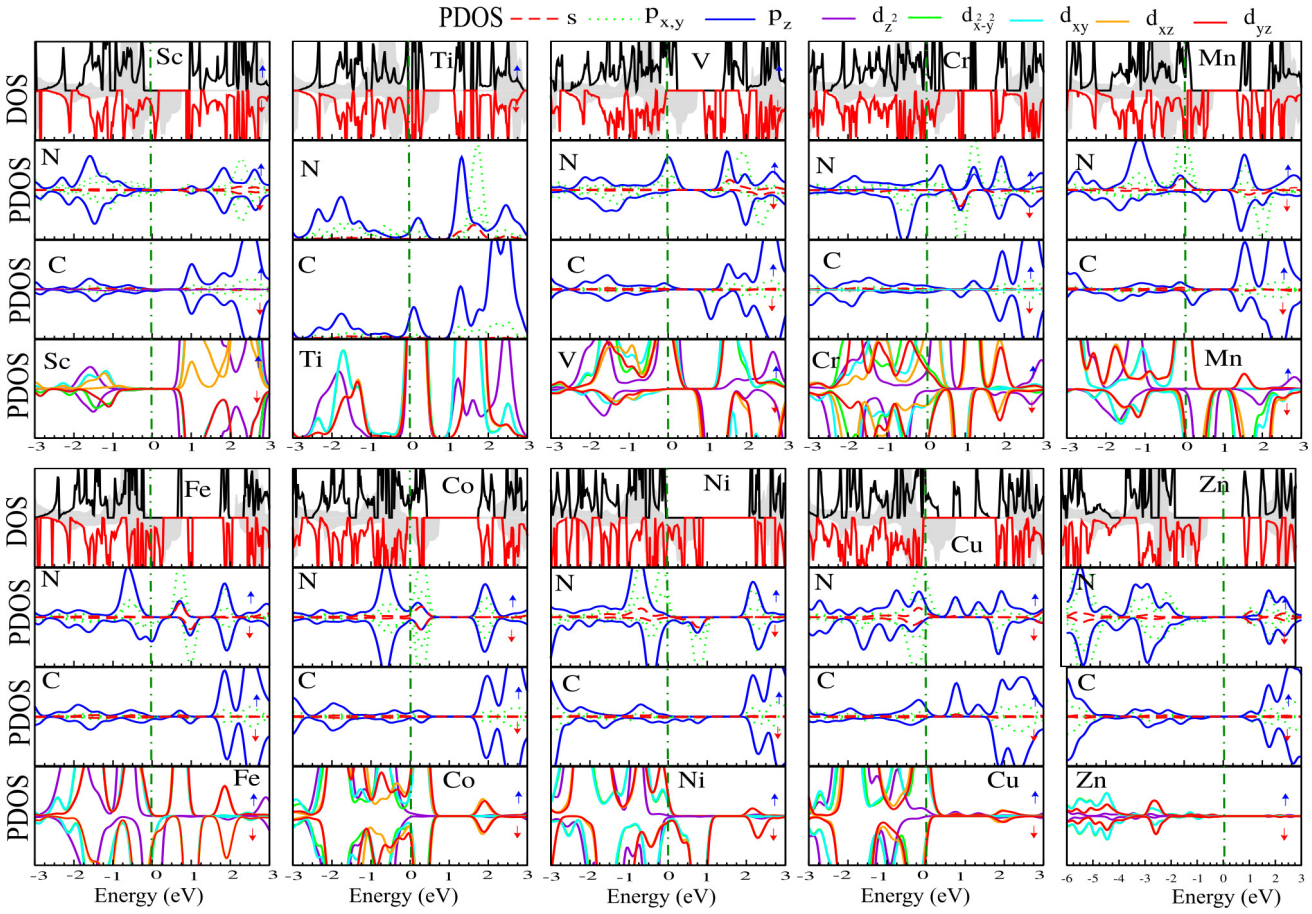

Figure S5: DOS and PDOS of Sc, Ti, V, Cr, Mn, Fe, Co, Ni and Zn atoms embedded into holey site of C_4N_3 nanosheet. The zero of energy is set at E_F as shown by the dashed green line.