Supporting Information for

Type-II Weyl fermion induced hydrogen adsorption in two-dimensional electride $[Ca_2N]^+ \cdot e^-$

Zeqing He, [1,2#] Weizhen Meng[1,2#], Ying Liu[1,2*], Xiaoming Zhang[1,2], and Guodong Liu[1,2*]

[1]*School of Materials Science and Engineering, Hebei University of Technology, Tianjin 300130, China.*

[2]*State Key Laboratory of Reliability and Intelligence of Electrical Equipment, Hebei University of Technology, Tianjin 300130, China.*

[#]*He and Meng are equal contribution in this work*

[*] E-mail of corresponding author: ying_liu@hebut.edu.cn; gdliu1978@126.com

Sec. A The absorption energy of bulk Ca_2N

In this section, we calculate the hydrogen adsorption energy for the bulk of the electride Ca_2N in Fig. S1. One could easily derive that the hydrogen adsorption energy eventually approaches -0.78 eV. This result is much smaller than that of monolayer Ca_2N (-0.97 eV). This result indirectly indicates the functions of the type-II Weyl point, it give rises to a positive influence on hydrogen adsorption process.

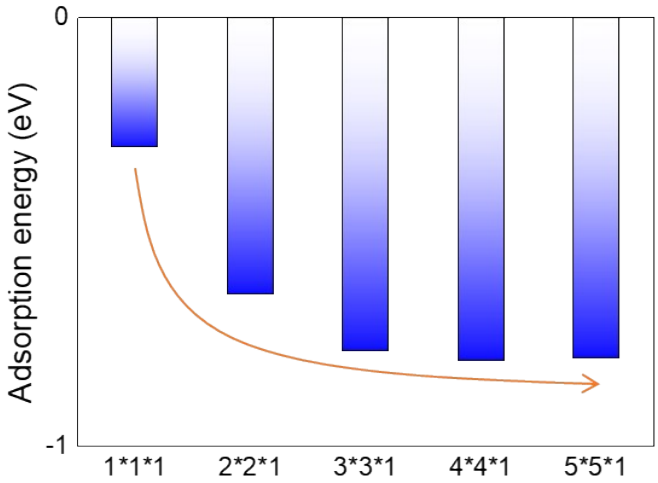

Fig. S1 Hydrogen adsorption energy of 1×1×1, 2×2×1, 3×3×1, 4×4×1 in bulk electride Ca_2N

Sec. B Electron localization function (ELF) with hole-doping

In this section, we calculate the electron localization function (ELF) of doping with 0~1 holes in electride Ca_2N in Fig. S2. We can find that the excess electrons are gradually neutralized with the doping of the hole. Then, we also calculate the electronic band structures of doping with 0-1 holes in electride Ca_2N in Fig. S3. With the increase of hole doping, Weyl fermions first approach and then move away from the Fermi level, where 0.4-holes are the critical point.

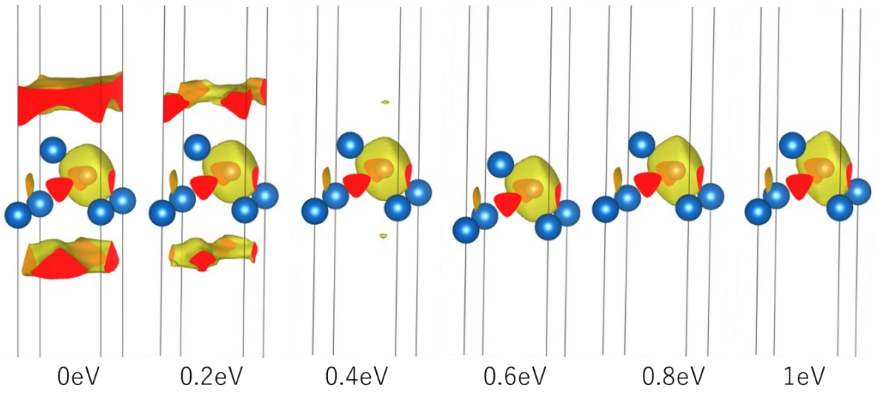

Fig. S2 The electron localization function (ELF) of doping with 0~1 holes in electride Ca_2N, with the isosurface values set as 0.6.

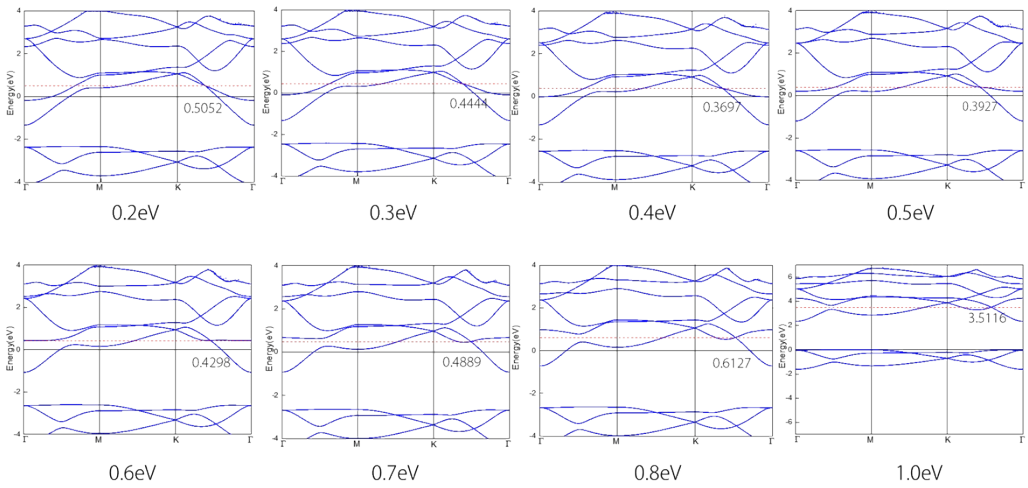

Fig. S3 Electronic band structures with doping holes (0~1) in electride Ca_2N. The red dashed line indicates the positions of the type-II Weyl point.

In this section, we calculate the electron localization function (ELF) under -6% ~ 6% strains in Fig. S4. We can find that the excess electrons always exist on both sides of Ca_2N. Then, we also calculate the electronic band structures under -6% ~ 6% strains in Fig. S5. The Weyl fermion is gradually approaching from the Fermi level under -6% ~ 6% strains.

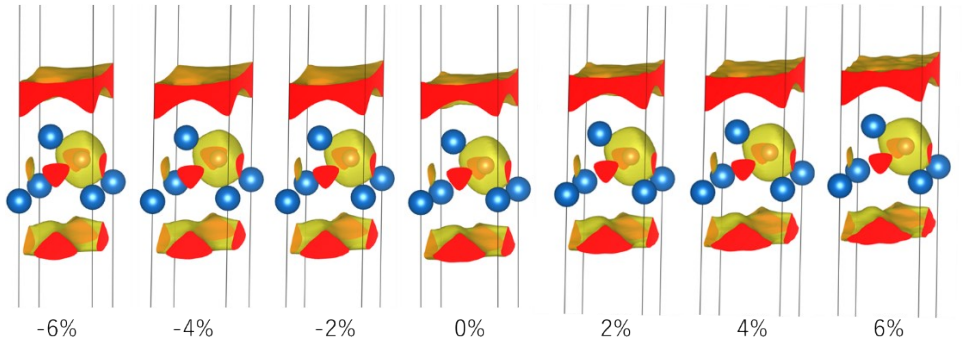

Fig. S4 The electron localization function (ELF) under -6% ~ 6% strains, with the isosurface values set as 0.6.

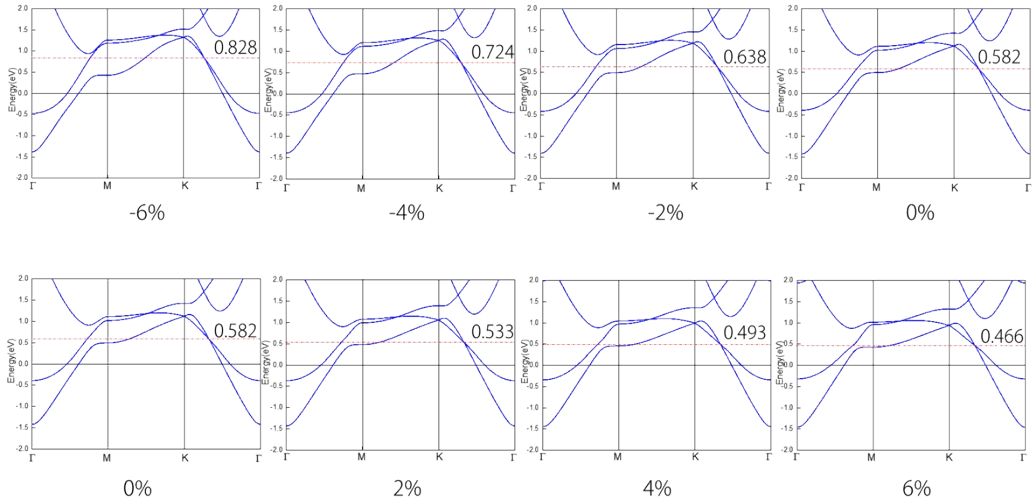

Fig. S5 The electronic band structure under -6% ~ 6% strains. Among them, the red line indicates the positions of the type-II Weyl point.

Sec. C Dynamical stability of 2D Ca2N under biaxial strains and Electronic band structure under uniaxial strains

The phonon energy spectra of electride Ca_2N under different biaxial strains (-6% ~6 %) are calculated, as shown in Fig. S6. We plot phonon energy spectra are calculated under the 5×5×1 supercell. One could observe that all phonon energy spectra have no virtual frequencies along the *k*-paths Γ-M-K- Γ. Therefore, the electride Ca_2N under biaxial strain (-6% ~6%) is dynamically stable.

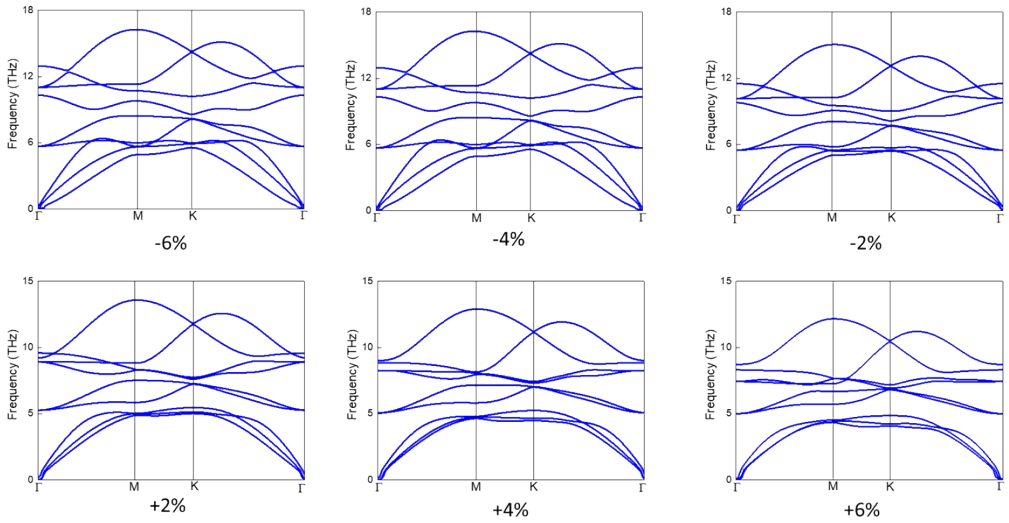

Fig. S6 Phonon energy spectra of electride Ca_2N under different biaxial strains (-6% ~6 %).

We find that the uniaxial strain could destroy the Weyl point on the K-Γ path, resulting in a gap a, as shown in Fig. S7.

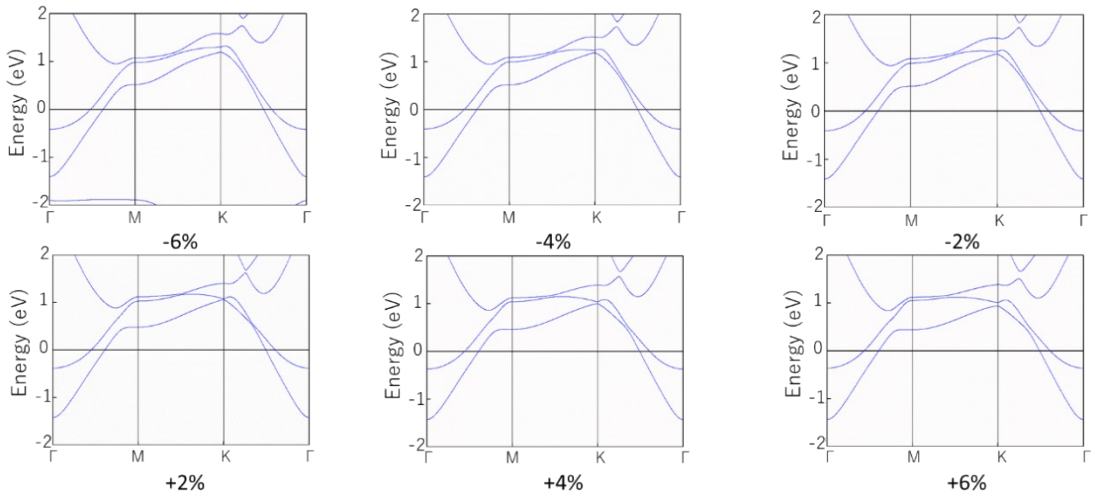

Fig. S7 The electronic band structure of uniaxial strain (-6 ~ 6%) in electride Ca_2N.

Sec. D Results for regulating strains under hole-doping

When we regulate strains under hole-doping, the positions of Weyl point gradually approach the Fermi level [Figs. S9-S14], and the hydrogen adsorption energy gradually increases, as shown in Fig. S8 (a-d) [See Table SI for specific values]. Therefore, these results indicate that the distance of the Weyl point from the Fermi level highly affects the hydrogen adsorption effect of Ca_2N.

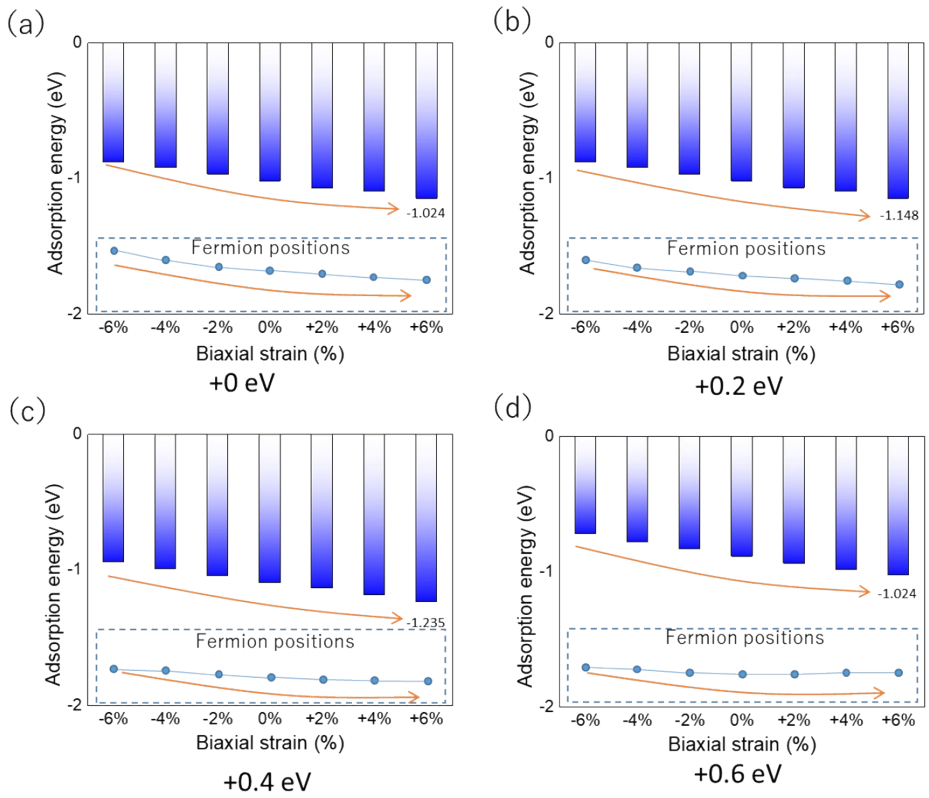

Fig. S8 (a-d) The hydrogen adsorption energy of different strain (-6% ~ 6%) under holes-doping (0~1 eV) in electride Ca_2N. In (a-d), the insets show the distance of Weyl point from the Fermi level.

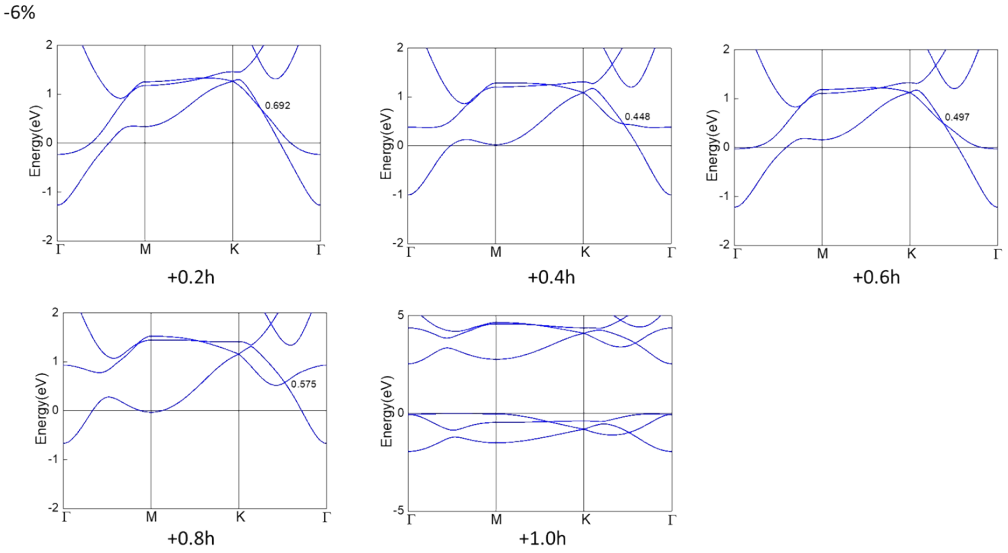

Fig. S9 The electronic band structures of different holes-doping under -6% strain.

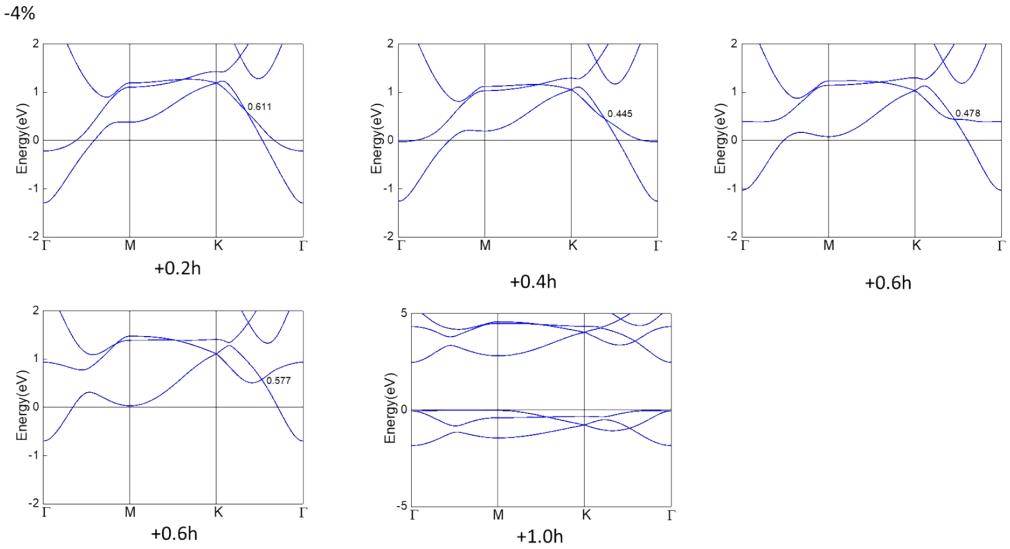

Fig. S10 Electronic band structures of different holes-doping under -4% strain.

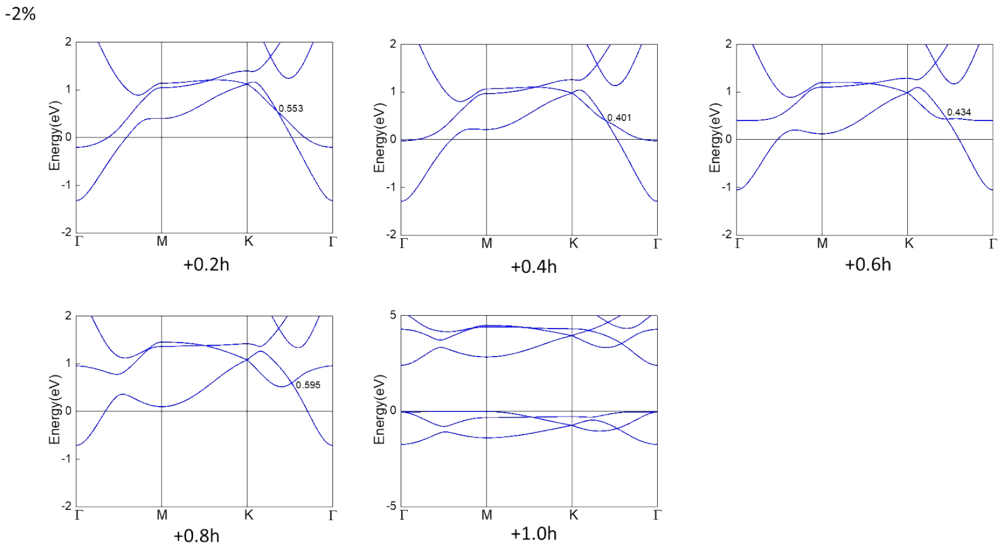

Fig. S11 Electronic band structures of different holes-doping under -2% strain.

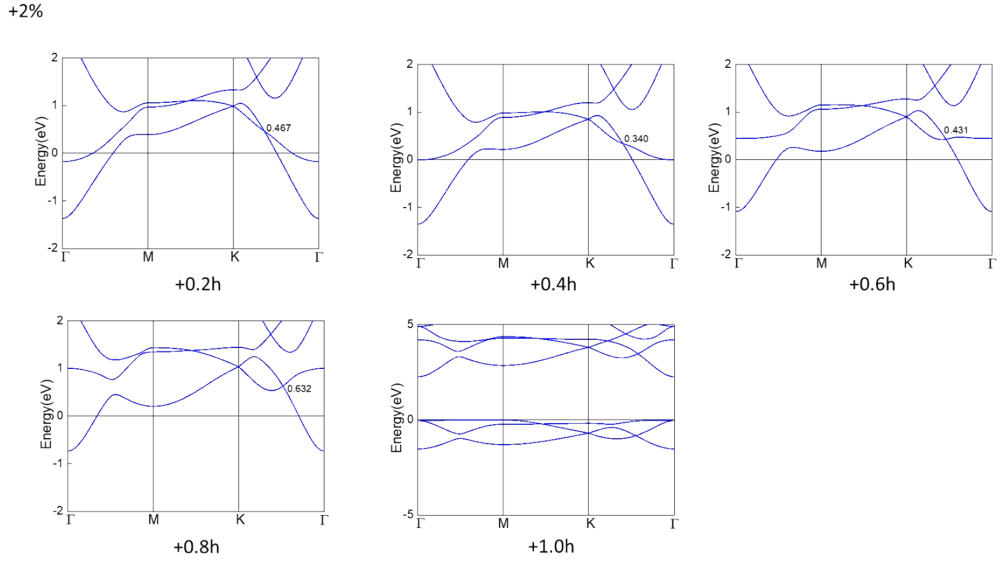

Fig. S12 Electronic band structures of different holes-doping under +2% strain.

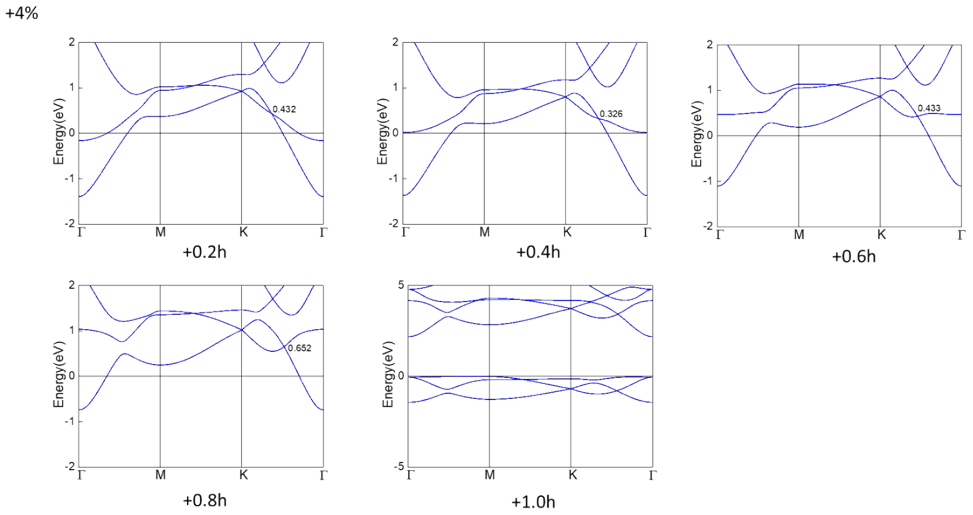

Fig. S13 Electronic band structures of different holes-doping under +4% strain.

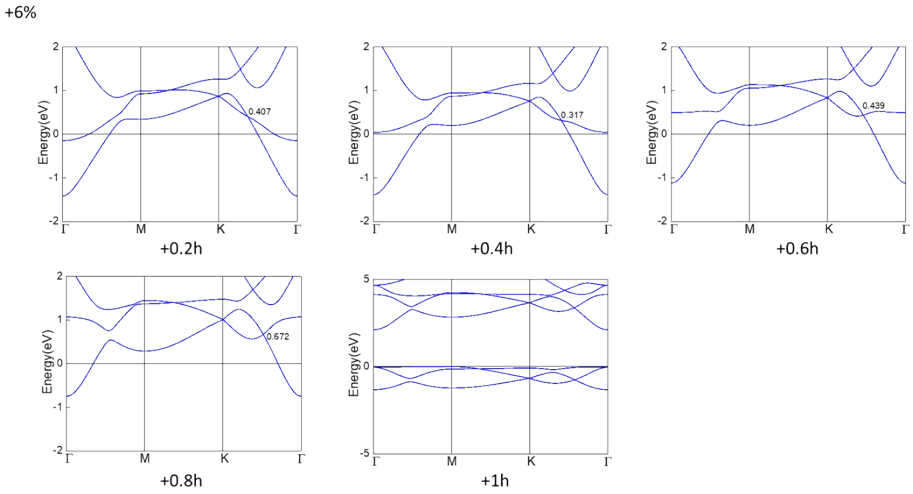

Fig. S14 Electronic band structures of different holes-doping under +6% strain.

Table SI: Adsorption energy of different strains (-6% ~ +6%) under holes-doping (0.2 eV ~ 1.0 eV)

Holes: 0.2 eV	
Strains	Adsorption energy (4*4*1)
-6	-0.87909
-4	-0.92289
-2	-0.97048
0	-1.01957
+2	-1.07132
+4	-1.09769
+6	-1.14764

Holes: 0.4 eV	
Strains	Adsorption energy (4*4*1)
-6	-0.94529
-4	-0.99629
-2	-1.04573
0	-1.0977
+2	-1.13597
+4	-1.18531
+6	-1.23513

Holes: 0.6 eV	
Strains	Adsorption energy (4*4*1)
-6	-0.7176
-4	-0.7797
-2	-0.83209
0	-0.88715
+2	-0.93902
+4	-0.98492
+6	-1.02445

Holes: 0.8 eV	
Strains	Adsorption energy (4*4*1)
-6	-0.47111
-4	-0.54774
-2	-0.60216
0	-0.66574
+2	-0.72326
+4	-0.76761
-6	-0.80474

Holes: 1.0 eV	
Strains	Adsorption energy (4*4*1)
-6	1.97414
-4	1.9825
-2	1.99919
0	1.9853
+2	1.9572
+4	1.92159
+6	1.87453

Sec. E Discussion of further adsorption of hydrogen atoms

The effect of the hydrogen adsorption in Ca_2NH is further discussed. First, when the hydrogen is adsorbed on the (001) surface of Ca_2N, the excess electrons are transferred to H on the surface, forming the conventional compound Ca_2NH, as shown in Fig. S15 (b,c). However, the electronic structure of Ca_2NH becomes the semiconductor, as shown in Fig. S15(a). In this case, we calculate the hydrogen adsorption energy of Ca_2NH, which is about -0.46191 eV. The results show that the hydrogen adsorption can still occur in Ca_2NH, which agree well with the results of Kitano et al. [Chem. Sci. 7, 4036 (2016)]. However, when hydrogen is further adsorbed on the (001) surface of Ca_2NH_2 compound, the adsorption energy is positive, indicating that no hydrogen adsorption occurs on Ca_2NH_2.

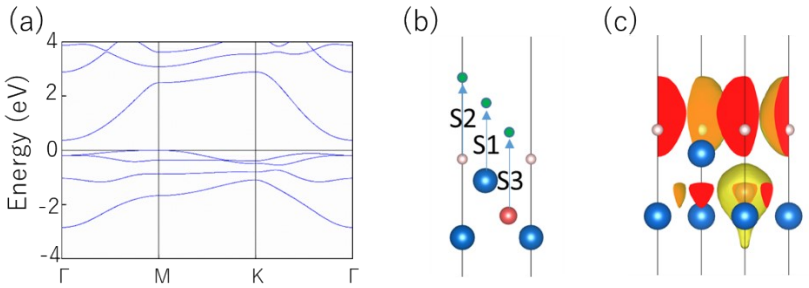

Fig. S15 The electronic structure of Ca_2NH. (b), (c) Indicates the crystal structure and ELF of Ca_2NH, respectively.