Supporting Information for

Oxidation, Stability, and Magnetic Ground States of Two-Dimensional Layered Electrides

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1. The configurations of O coverage on Ca_2N and Y_2C

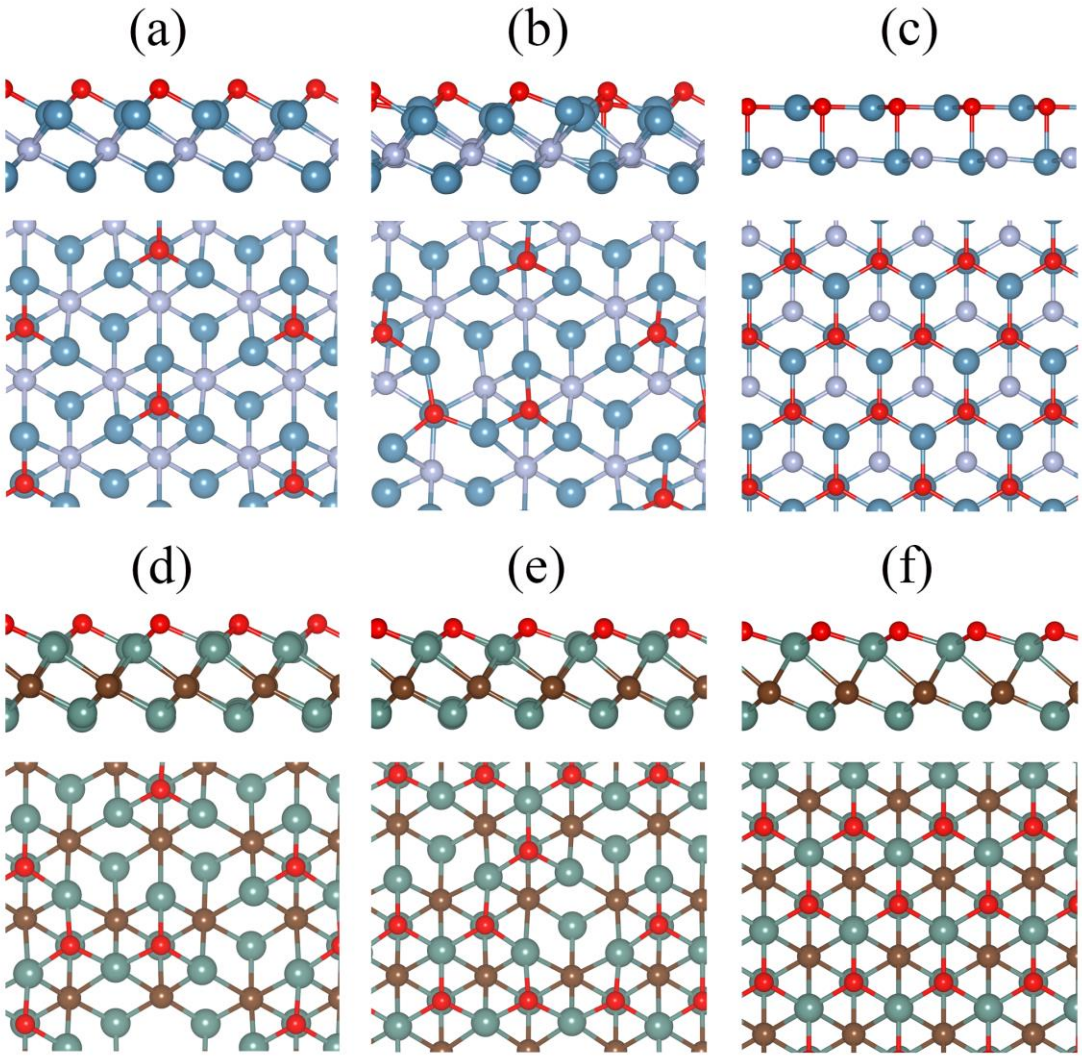

Figure S1. Side (upper) and top (lower) views of the O-terminated Ca_2N monolayer in (a) 3/9 ML, (b) 4/9 ML, (c) 1 ML; O-terminated Y_2C monolayer in (d) 4/9 ML, (e) 6/9 ML, (f) 1 ML. In (b),(e), the changes in the bond lengths and angles are 0.34 Å and 15.5° for Ca_2N and 0.16 Å and 6.1° for Y_2C.

2. The projected density of states (PDOS) of Ca_2N and Y_2C

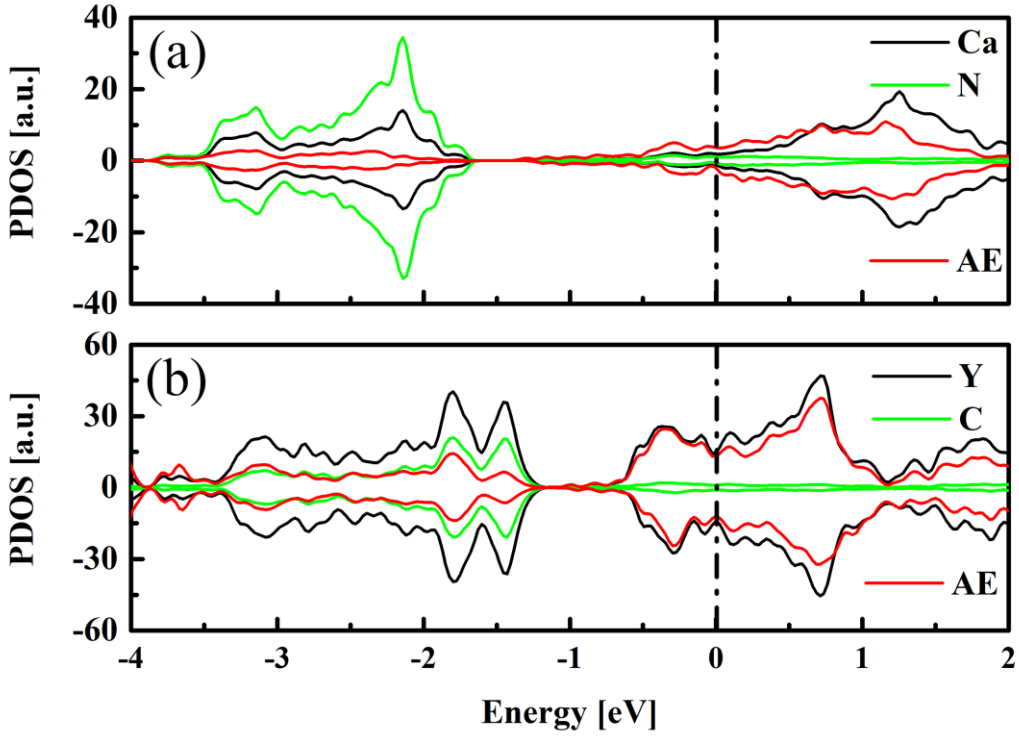

Figure S2. The projected density of states (PDOS) of (a) Ca_2N and (b) Y_2C. The "AE" indicate the surface anionic electrons. The zero energy references represent the Fermi level of each system.

3. The integrated magnetic moments of the O-adsorbed electrides

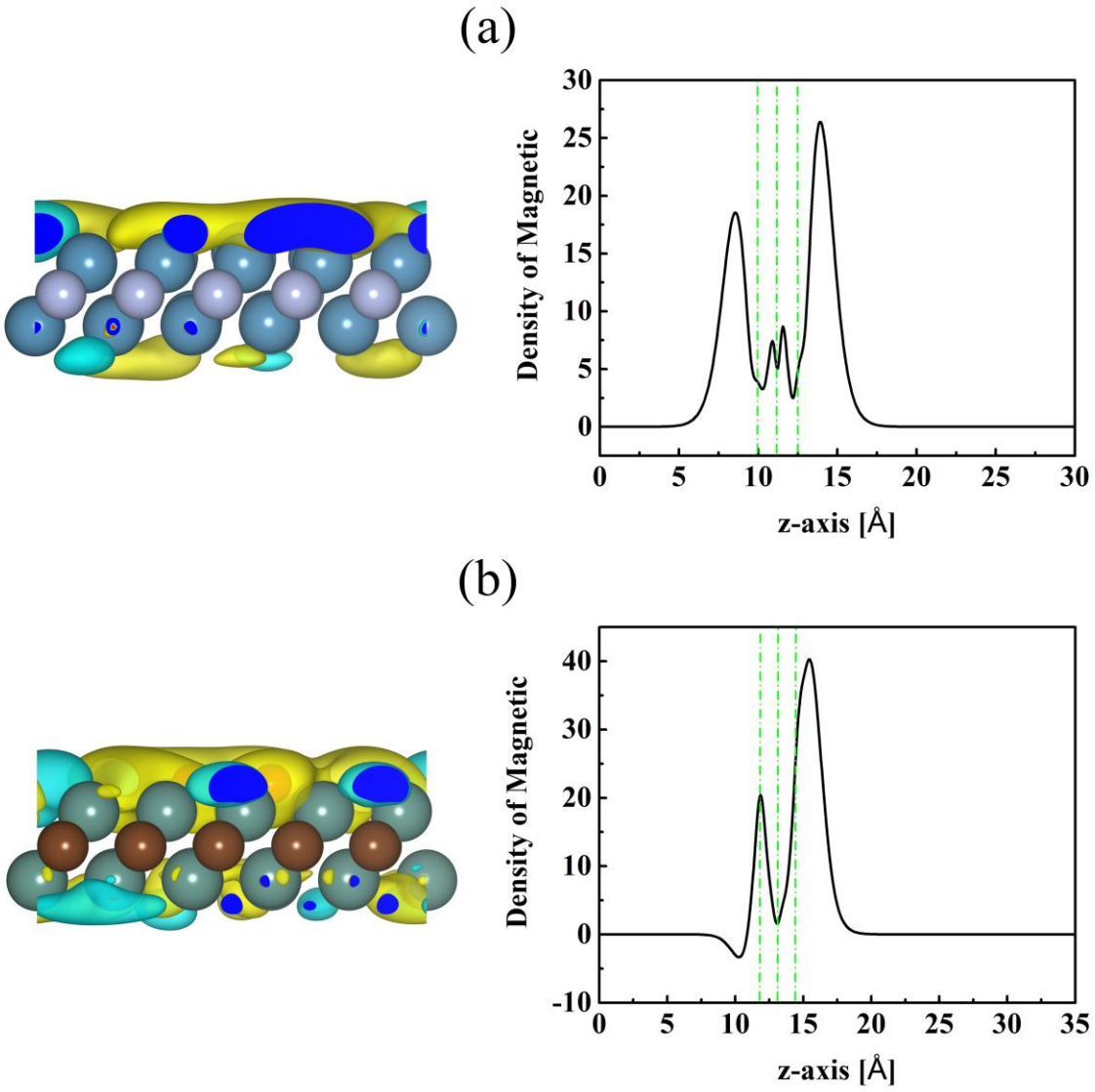

Figure S3. The side view of the spin density (left) and the integrated magnetic moments of the O-adsorbed (a) Ca_2N and (b) Y_2C. The dashed lines in the graphs indicate the positions of the atomic layers. The spin densities were drawn with an isosurface of 0.0008 *e*/bohr^3 for Ca_2N and Y_2C.

4. The spin density of the O monomer case in Ca_2N and Y_2C

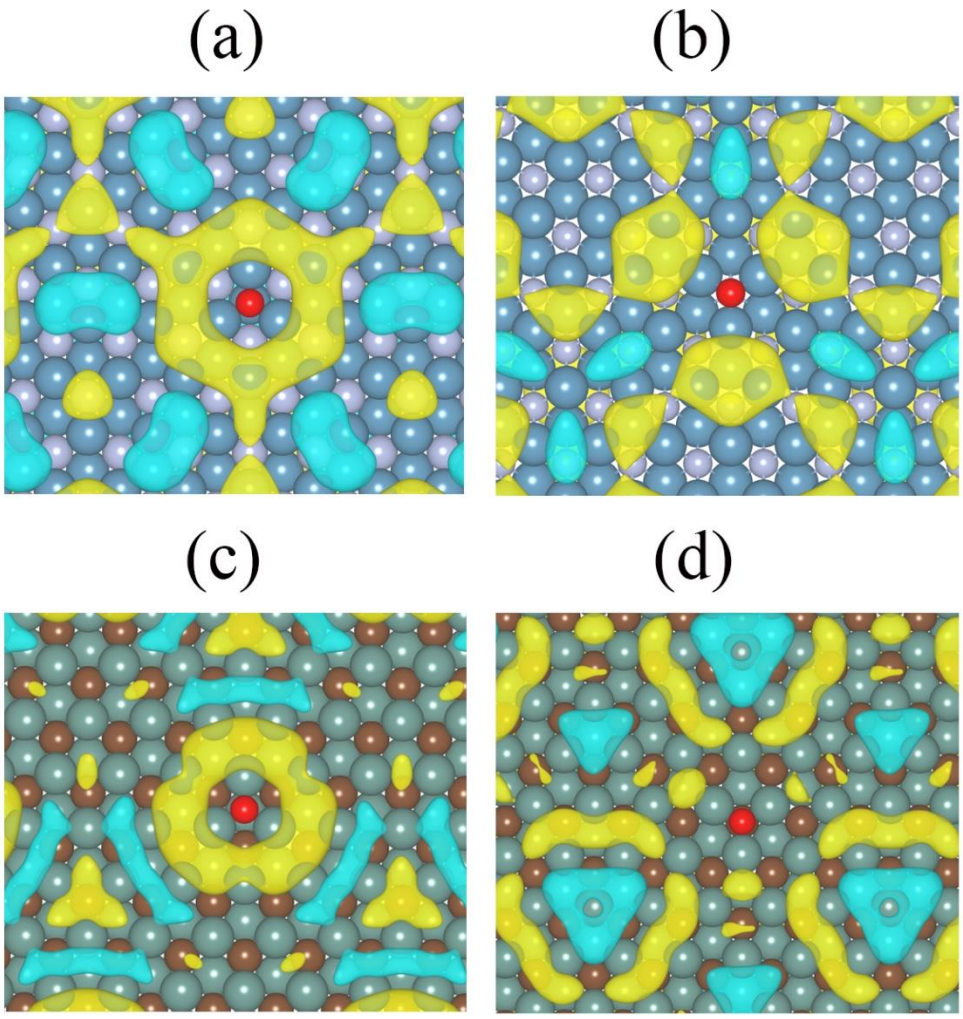

Figure S4. The spin density of O monomer adsorption on (a) h1 and (b) h2 sites for Ca_2N and (c) h1 and (d) h2 sites for Y_2C. The isosurfaces were taken at 0.0008 *e*/bohr^3.

5. The spin density of the vacancy case in Ca_2N and Y_2C

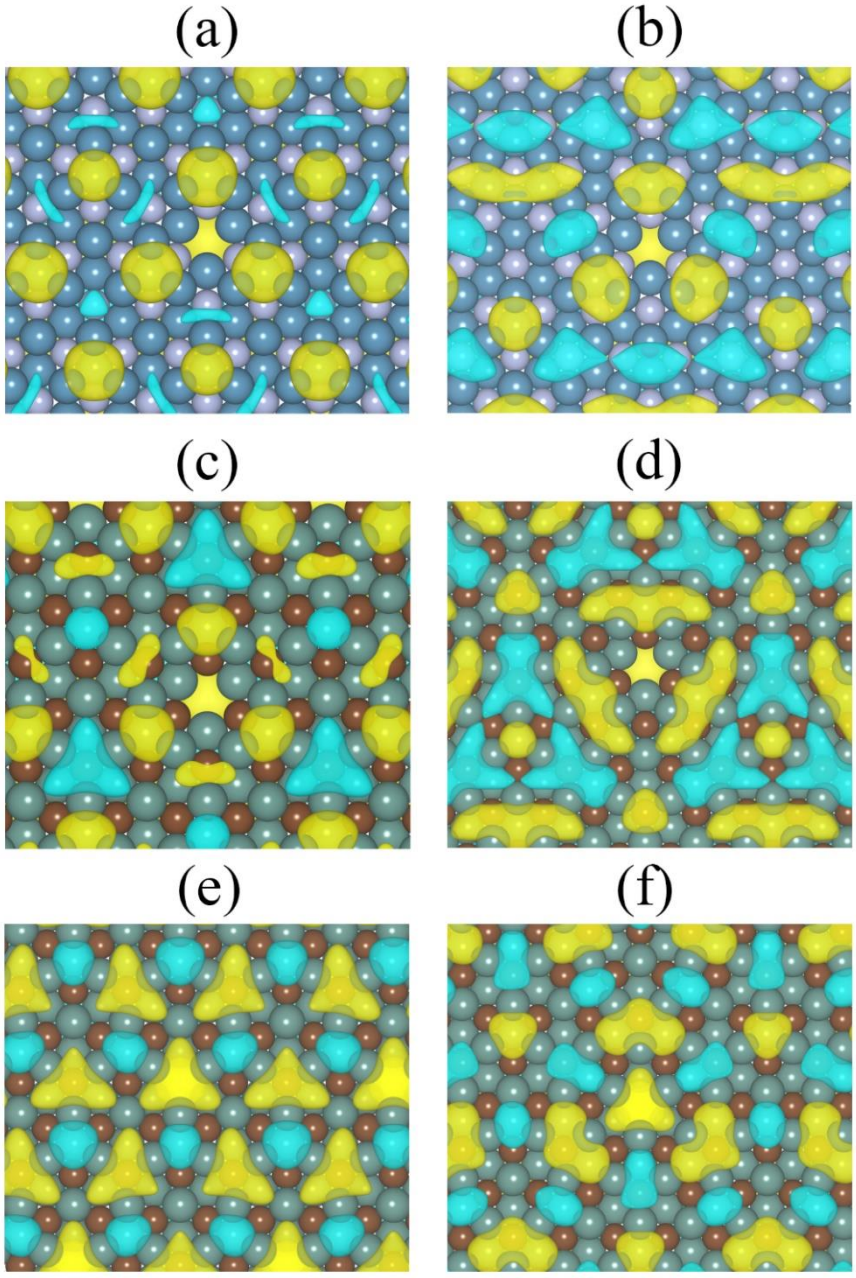

Figure S5. The spin density of (a, b) Ca vacancy in Ca_2N, (c, d) Y vacancy and (e,f) C vacancy in Y_2C for 4×4×1 and 5×5×1 supercell. The spin densities were drawn with an isosurface of 0.0008 e/bohr^3 for Ca_2N and 0.0015 e/bohr^3 for Y_2C.

6. The differential charge density and spin density of bilayer and trilayer Ca_2N

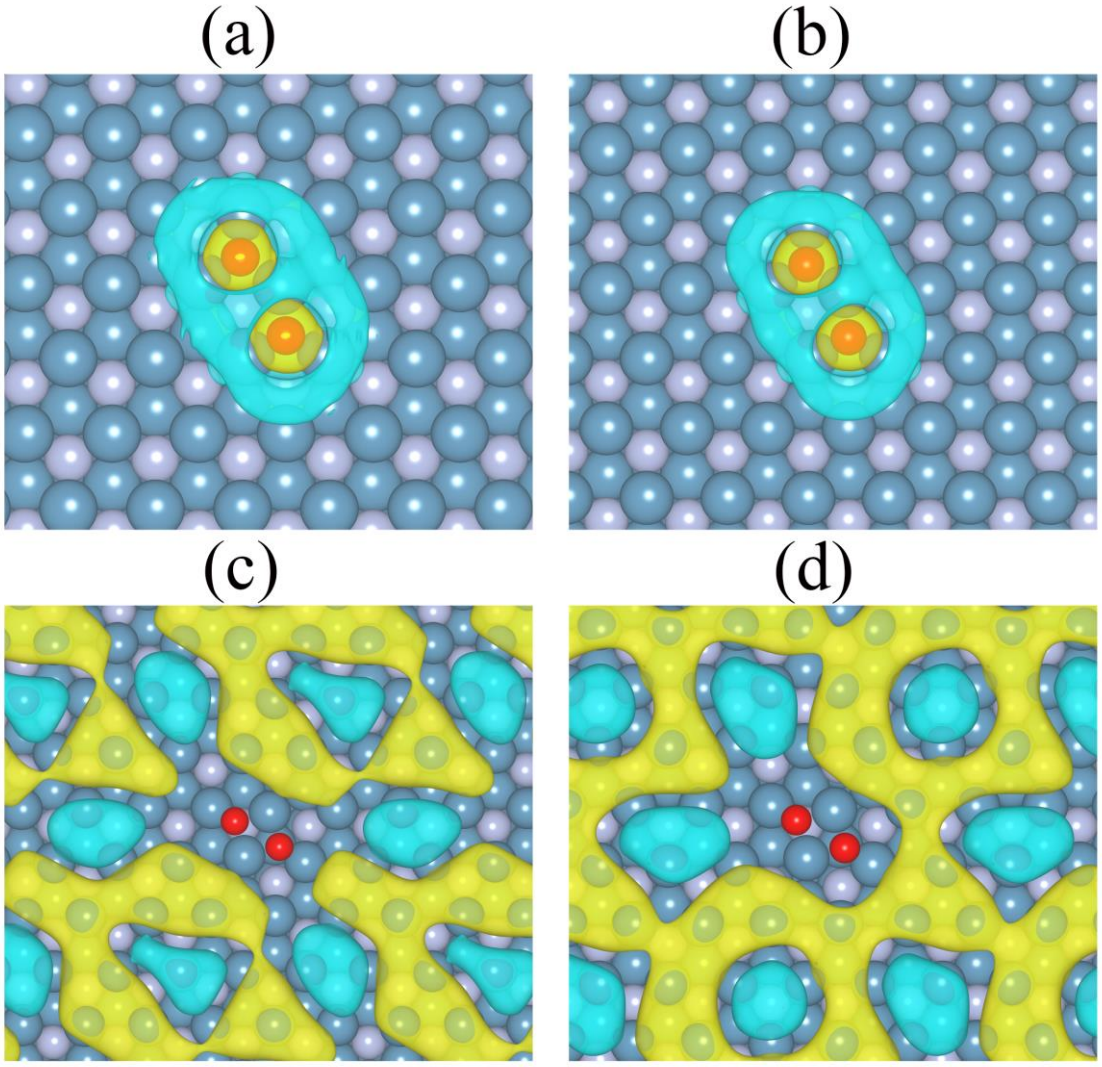

Figure S6. The differential charge density and spin density of (a,c) bilayer Ca_2N and (b,d) trilayer Ca_2N. The isosurfaces were taken at a charge density 0.001 *e*/bohr^3 for differential charge density and 0.0003 *e*/bohr^3 for spin density.

7. The partial density of states of bilayer and trilayer Ca_2N

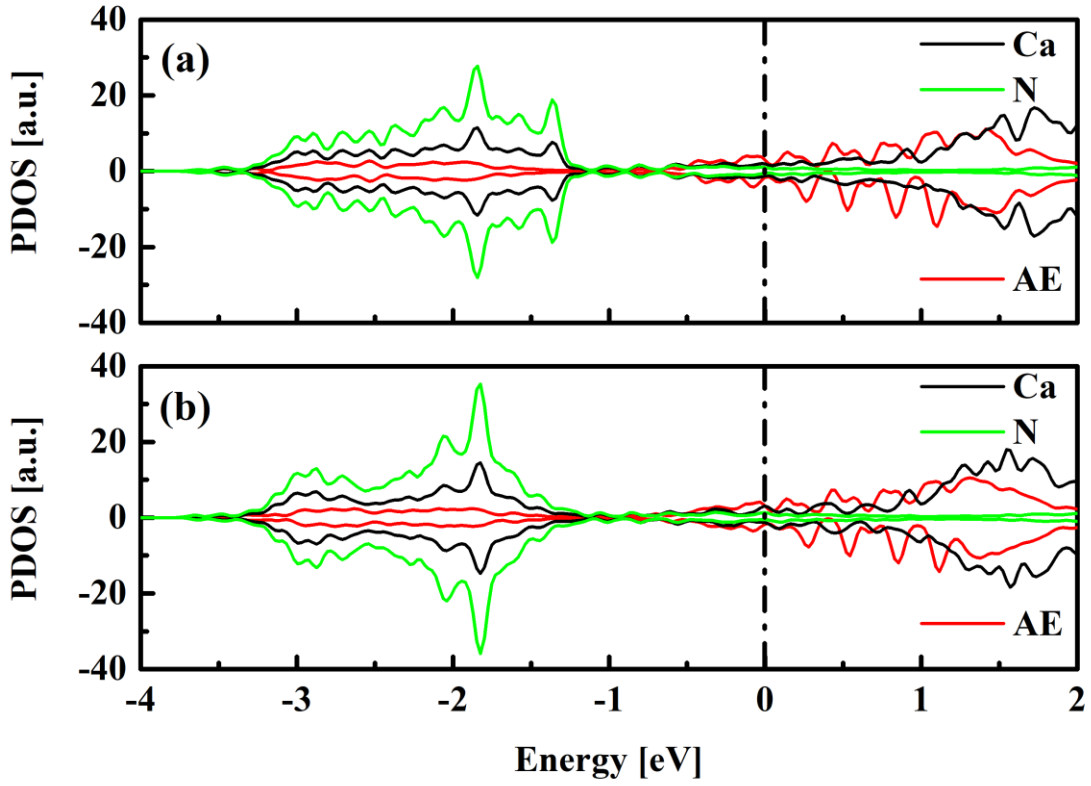

Figure S7. The projected density of states (PDOS) of (a) bilayer Ca_2N and (b) trilayer Ca_2N. The red line of AE stand for surface anionic electrons. The zero energy references represent the Fermi level of each system.

8. The data of oxygen monomers with different distance

Table S1. The adsorption energy, magnetic moment and charge transfer of oxygen monomers with different distance (Å) in Ca_2N and Y_2C. The units are eV, μB and e, respectively.

Ca_2N	Distance [Å]	Adsorption E [eV]	Magnetic M [μB]	Transfer Charge [e]
	3.591	-4.842	0.14	1.43
	6.220	-4.906	0.10	1.42
	12.440	-4.925	0.13	1.43
	17.955	-4.951	0.10	1.44
Y_2C	Distance	Adsorption E	Magnetic M	Transfer Charge
	3.520	-5.625	0.13	1.37
	6.099	-5.602	0.12	1.38
	12.198	-5.580	0.07	1.38
	17.600	-5.591	0.04	1.38