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Supplementary Information

for

Two-Dimensional [CaCl]+•e- and its strippable feasibility as an applicable electride with room temperature ferromagnetism and extremely low work function

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Table SI shows the values of magnetic moment (μ_B) and work function (eV) with the change of layer spacing ($d_{CaCl\text{-}graphene}$).

$d_{CaCl\text{-}graphene}$ (Å)	Magnetic moment (μ_B)	Work function (eV)	$d_{CaCl\text{-}graphene}$ (Å)	Magnetic moment (μ_B)	Work function (eV)
2.5	0	2.9079	4.3	0.382	3.4127
2.8	0	2.9313	4.6	0.9733	3.4479
3.1	0	3.0443	4.9	0.9542	3.4533
3.4	0.1739	3.1736	5.2	0.96	3.4567
3.7	0.2725	3.2643	5.5	0.956	3.4543
4.0	0.3182	3.2719	6.0	0.9643	3.4573

We plotted the charge difference density of electride CaCl, as shown in Figure S1. We found that Ca did lose electrons, some of them to Cl, some of them to the lattice cavity.

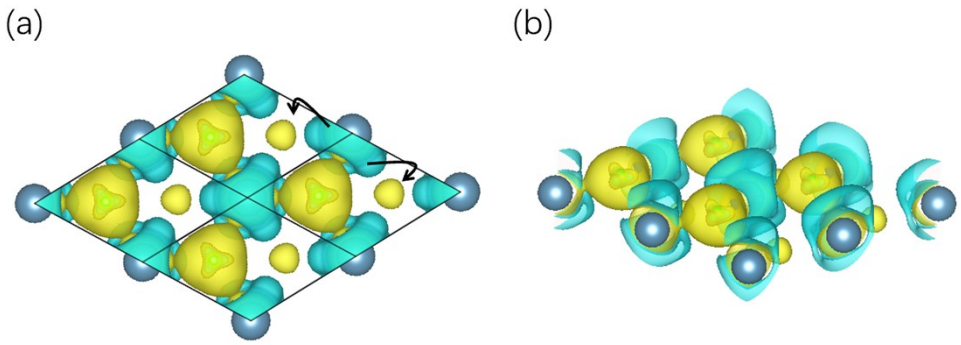

Fig. S1 (a) and (b) show the charge difference density of electride CaCl, where the green and yellow shades represent lost and gained electrons, respectively.

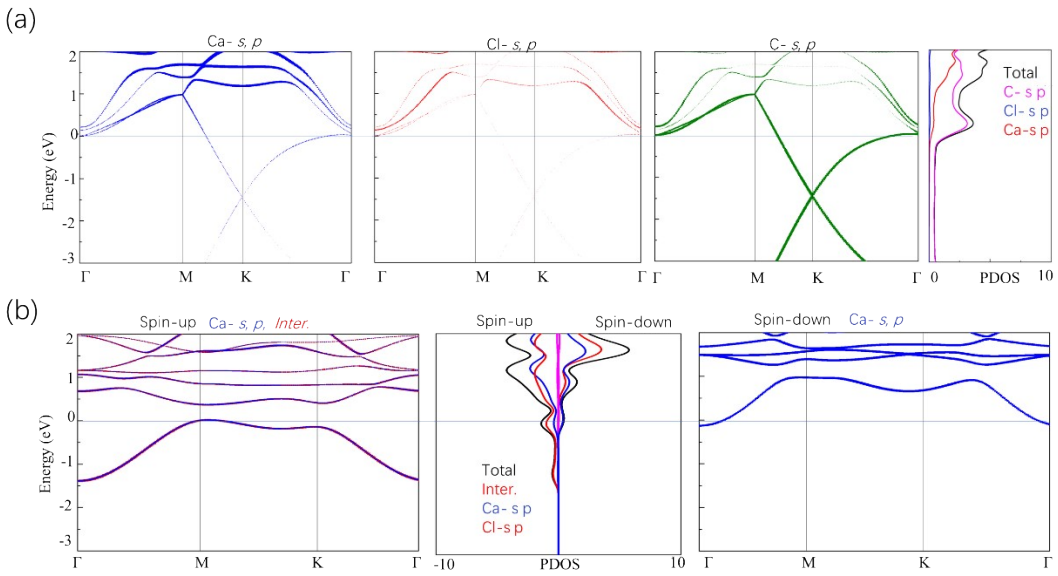

Fig. S 2 (a) and (b) show the orbital projection and PDOS of CaCl/ Graphene and monolayer CaCl

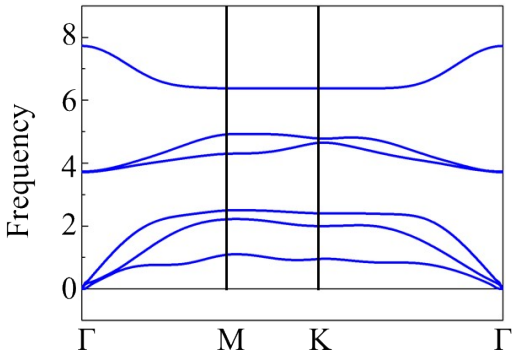

Fig. S 3 shows phonon spectrum of monolayer CaCl.

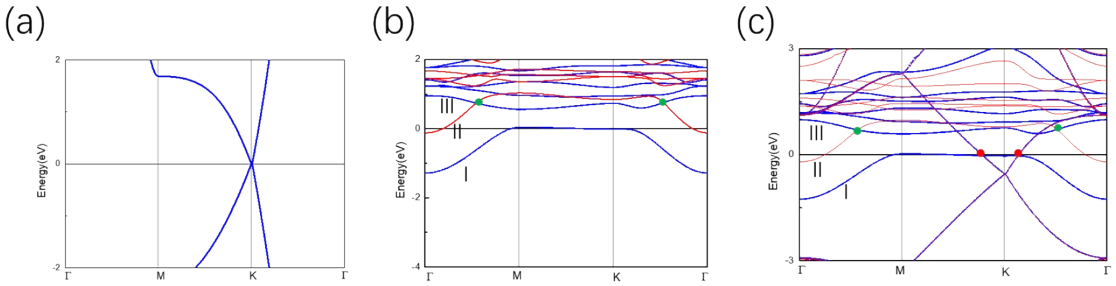

Fig. S 4 (a), (b), and (c) show electronic band structure of monolayer graphene, CaCl, CaCl/graphene.

Then, the thermodynamic and kinetic stability of CaCl/graphene under $d_{CaCl\text{-}graphene}$ = 5 Å are shown in Fig. S 5 (a, b). In dynamic stability, we find that there is

almost no virtual frequency on other K paths except for a little virtual frequency near the Γ point. In thermodynamics, we find that the final crystal structure of CaCl/graphene under 300 K has poor stability. In other words, when the distance between the graphene and CaCl is larger than 4 Å, CaCl/graphene is dynamically stable.

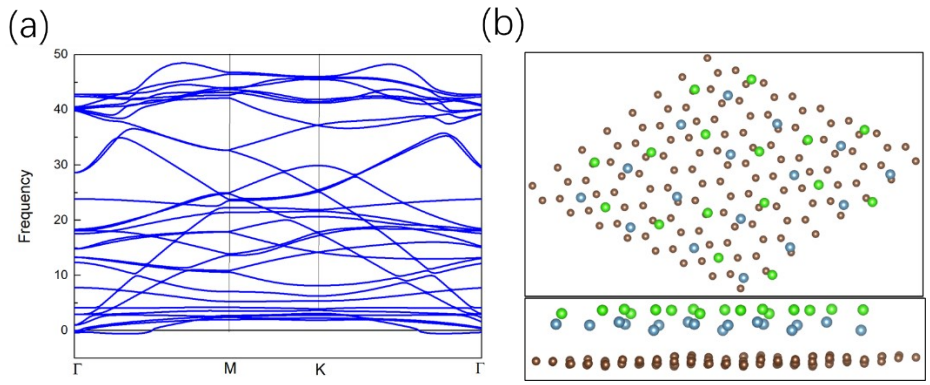

Fig. S 5 (a) and (b) show the thermodynamic and kinetic stability of CaCl/graphene under $d_{CaCl\text{-}graphene}$ = 5 Å