Supporting Information

Topological Phases in Hydrogenated Group 13 Monolayers

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Crystal structure of gallenane analogous group 13 sheets

Aluminane, indinane and thallinane are the analogous group 13 elements of gallenane. All these 2D sheets have orthorhombic space group $Pbcm$. The structural informations of all these systems are given in Table S1. The lattice parameter and buckling height increase from aluminane to thallinane, whereas gallenane has lower buckling height than aluminane. The M–M bond lengths also increase from aluminane to thallinane as shown in Table S1, column 7–9, however gallenane has lower M–M than aluminane. The shortest bond length indicates enhanced interaction between two metal sites in aluminane as compared to other group 13 elements. Also, the M–H bond length increase from aluminane to thallinane as shown in Table S1, coulumn 10. Dynamical stability of all sheets and strain gallenane are verified by the phonon band structures as shown in Figure S1.

Table S1: Structural parameters of gallenane analogous group 13 sheets

M	a (Å)	b (Å)	d (Å)	θ_1 (°)	θ_2 (°)	$d_{M_1-M_2}$ (Å)	$d_{M_2-M_3}$ (Å)	$d_{M_2-M_4}$ (Å)	d_{M-H} (Å)
Al	4.50	4.72	1.41	61.74	86.77	2.75	2.82	2.74	1.59
In	5.14	5.32	1.49	61.74	87.63	3.05	3.23	3.05	1.73
Tl	5.25	5.60	1.62	74.50	74.90	3.24	3.85	3.86	1.78

Table S2: Binding energies of the nodal fermions in the absence of SOC and gaps at the nodal points in the presence of SOC

M	NP_1 [meV]	NP_2 [meV]	$\Delta E_{NP_1}(\text{SOC})$ [meV]	$\Delta E_{NP_2}(\text{SOC})$ [meV]
Al	71	-39	0	0
Ga	54	-21	29	21
In	176	-27	74	104
Tl	243	-118	77	213

All the 2D hydrogenated group 13 sheets except borophane, exhibit a nodal ring in the absence of SOC, consisting of two nodal points (NP_1 and NP_2) near the Fermi level. The binding energies of nodal fermions are shown in Table S2, where the energies are calculated with respect to Fermi level. In the presence of

Figure S1: Phonon band structures of (a) aluminane, (b) indinane, (c) thallinane and (d) gallenane at -2.6% strain

SOC, a small gap opens at the nodal points in all hydrogenated group 13 sheets, apart from aluminane. The gaps at NP_1 and NP_2 for all of these structures are tabulated in Table S2. From Table S2, we can infer that gap opening at NP_1 and NP_2 increase on going from gallene to thalline. It could be due to the prominent relativistic effects in the heavier group 13 elements.

Indinane and thallinane

Figure S2: (a) Orbital resolved electronic band structure of indinane without inclusion of SOC, (b) and (d) edge states along (010) direction and bulk gap spectral function on k-plane respectively. (c) orbital resolved band structure of indinane with the inclusion of SOC

Figure S2(a) shows the band structure of indinane without inclusion of SOC. It also shares same topological NLSM features as that of gallene. The nodal ring in indinane is formed from the contribution of s and p orbitals of indium as shown in Figure S2(a). We have simulated the ARPES of edge states along

the (010) direction as shown in Figure S2(b). The gap spectral function on a k-plane near the Fermi level is shown in Figure S2(d), comprises of two closed loop. With the incorporation of SOC, indinane opens a gap at two nodal points as shown in Figure S2(c).

Thallium is the heaviest group 13 element. Its hydrogenated monolayer i.e. thallinane also shows topological NLSM with two linear band crossing along Y- Γ as shown in Figure S3(a). It has an additional linear band crossing along Γ -X. Drumhead edge states of thallinane are shown in the Figure S3(b), which contains bright yellow line connecting two nodal points. The nodal loop of thallinane is slightly different from other hydrogenated group 13 sheets as shown in Figure S3(d), which involve two nodal loop connected by the lines. Electronic band structure of thallinane in the presence of SOC is shown in Figure S3(c). The nodal gap of thallinane, in the presence of SOC is highest among all hydrogenated group 13 sheets.

Figure S3: (a) Orbital resolved electronic band structure of thallinane without inclusion of SOC, (b) and (d) edge states along (100) direction and bulk gap spectral function on k-plane, respectively. (c) orbital resolved band structure of thallinane with the inclusion of SOC

Mirror symmetry protected gallenane

NLSM behavior of gallenane could be verified by breaking the symmetries. We have shifted one hydrogenated gallium atom from mirror plane as shown in Figure S4(a). So the glide $\{M_z|b/2\}$ and mirror $\{M_x|0\}$ symmetry of the system gets broken and nodal points are gapped as shown in Figure S4(b). In order to confirm the symmetry protection of the nodal points, we break the glide symmetry of parent structure by shifting one hydrogenated gallium atom along the c-direction, shown in Figure S4(c). Nodal points are still protected due to the mirror symmetry as shown in Figure S4(d).

Figure S4: (a) and (b) show gallenane crystal and electronic structure, respectively, with broken mirror and glide symmetries, (c) and (d) show gallenane crystal and electronic structure, respectively, with mirror symmetry only.

Band structure of hydrogenated group 13 monolayers with HSE06

Figure S5: (a), (b), (c) and (d) show the HSE band structure of aluminane, gallenane, indinane and thallinane respectively

Group theory analysis

A qualitative investigation of symmetry in the gallenane is performed by group theory analysis.^{1,2} The space group D_{2h}^{11} or $Pbcm$ contains little point groups at its high symmetric (HS) points and lines. These little point groups at HS points and lines listed in Table S3. All the HS points have full point group symmetry i.e., D_{2h} (mmm) of the space group D_{2h}^{11} and HS lines have C_{2v} (mm2) point group symmetry. The character table of D_{2h} (mmm) point group is shown in Table S4. We represent all the irreducible representation at Γ by Γ_i s. Where, “+” and “-” denote symmetric and anti-symmetric with respect to center of symmetry, respectively. Table S5 show the character table for the little point group $C_{2v}(\Delta)$. Figure S6 shows electronic band structure

of gallenane along Y to Γ with irreducible representation of all the bands. Although the little point group at Y point contains only the one dimensional representations, but still double degeneracy is present due to the non-symmorphic symmetry of the system. Along Y to Γ , little point group symmetry is $C_{2v}(\Delta)$ which also contains only one dimensional representation. So, the degeneracy along this path is accidental and preserved due to the presence of mirror symmetry,³ which is also verified by removing the symmetries as shown in Figure S4.

Figure S6: Shows the band structure of gallenane along Y to Γ with irreducible representations.

Table S3: Little point groups at all HS points and lines of Brillouin zone

HS points and lines	k	Little points group
Γ	(0,0)	D_{2h} (mmm)
X	$(\pi,0)$	D_{2h} (mmm)
S	(π, π)	D_{2h} (mmm)
Y	$(0,\pi)$	D_{2h} (mmm)
$\Sigma(\Gamma X)$	$(k_x,0)$	C_{2v} (mm2)
D (XS)	(k_x, π)	C_{2v} (mm2)
C (SY)	(π,k_y)	C_{2v} (mm2)
Δ (Y Γ)	$(k_y,0)$	C_{2v} (mm2)

Table S4: Charcter table for D_{2h} point group at Γ and Γ_i s are the irreducible representation.

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$	Basis function
Γ_1^+	1	1	1	1	1	1	1	1	s, d_{z^2} , $d_{x^2-y^2}$
Γ_2^+	1	-1	1	-1	1	-1	1	-1	d_{zx}
Γ_3^+	1	1	-1	-1	1	1	-1	-1	d_{xy}
Γ_4^+	1	-1	-1	1	1	-1	-1	1	d_{yz}
Γ_1^-	1	1	1	1	-1	-1	-1	-1	f_{xyz}
Γ_2^-	1	-1	1	-1	-1	1	-1	1	p_y
Γ_3^-	1	1	-1	-1	-1	-1	1	1	p_z
Γ_4^-	1	-1	-1	1	-1	1	1	-1	p_x

Table S5: Charcter table of the for Δ

Δ	E	$C_2(z)$	$\sigma_v(xz)$	$\sigma_v(yz)$	Basis function
Δ_1	1	1	1	1	p_z
Δ_2	1	1	-1	-1	
Δ_3	1	-1	1	-1	p_x
Δ_4	1	-1	-1	1	p_y

References

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