Supplementary Information

Topological insulator states in a honeycomb lattice of s-triazines

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This SI is meant to support the explanations described in the main text entitled "***Topological insulator states in a honeycomb lattice of s-triazines***". In the first part, we adopted a simple ruby TB model to describe the four valence bands of the g-C_6N_6 lattice nearest to the Fermi level and support the rationality of our TB model employed in the main text. In the second part, the four time-reversal momenta of g-C_6N_6 lattice from the corresponding electron Kohn-Sham wavefunctions are presented. In the last part, we calculated the phonon spectra of the g-$C_{12}N_6$ and g-$C_{24}N_6H_{12}$ to confirm their kinetic stability.

Part I. Ruby model

As described in main text, the configuration of the Kohn-Sham wavefunctions (Fig. 3(d)) display the features of a ruby lattice[1]. So we adopted a simple ruby TB model to reproduce the top four valence bands of the g-C_6N_6 lattice. Different from the TB model adopted in the main text, only one sp^2-hybridizatized orbital at each nitrogen atom was considered in this model, leading to six orbitals per unit cell. The effective Hamiltonian is written as:

$$H = \varepsilon \sum_i c_i^+ c_i + t \sum_{\langle i,j \rangle} c_i^+ c_j + \gamma \sum_{\langle\langle i',j' \rangle\rangle} c_{i'}^+ c_{j'}$$

where ε denotes the on-site energy of the sp^2-hybridizatized orbital, c_i^+ and c_i are the creation and annihilation operators of an electron on the i-th atom, respectively. The

parameters of t and γ are nearest-neighbor (NN) hopping parameters, as indicated in Fig. S1(a). When the parameters are set to ε=-1.745 eV, t=-0.80 eV and γ=-0.42 eV, this TB Hamiltonian reproduces well the four valence bands of the g-C_6N_6 lattice given by DFT calculations, especially the appearance of the Dirac cones as showed in Fig. S1(b). It was found that both TB models agree well with the DFT results. The slight deviation of the TB models to the DFT data can be attributed to the contribution of the atomic orbitals of carbon atoms, which was omitted in both TB models.

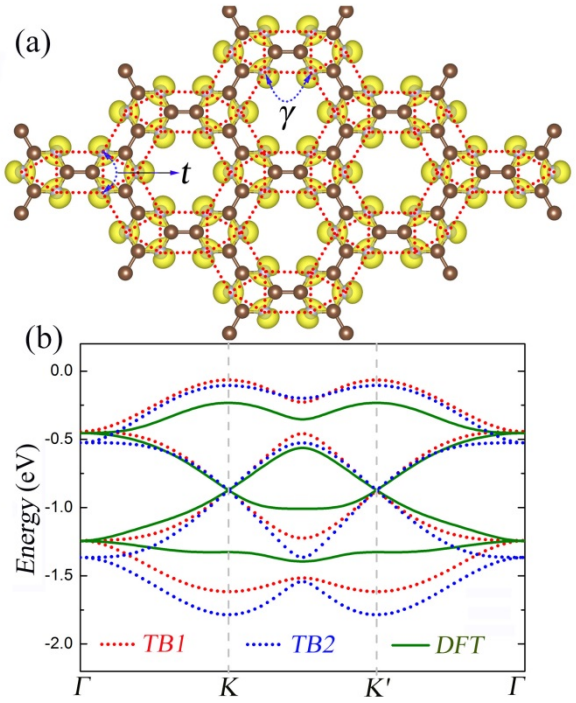

Fig. S1 (a) The isosurfaces of the Kohn-Sham wave functions of the four valence bands nearest to the Fermi level. The nearest neighbor hopping energy (t) between adjacent hexagons and the nearest neighbor hopping energy (γ) within the same hexagon of the N atoms are also indicated in the Figure. (b) Band structures obtained from two TB models and DFT calculations: TB1 involves p_x and p_y atomic orbitals of nitrogen atom (details in main text), TB2 has one sp^2-hybridizatized orbital at each nitrogen atom (Ruby model).

Part II. Parity tables for the g-C_6N_6 lattice and the corresponding Z_2 invariants

To confirm the topological nontriviality of the g-C_6N_6 lattice, we calculated the Z_2 topological invariants from the parities of the bands, according to the strategy proposed by Fu and Kane. The parities of the bands at the four time-reversal momenta: Γ (0, 0), M (1/2, 0), M (0, 1/2) and M (1/2, 1/2) are calculated from the Kohn-Sham electron wavefunctions obtained from DFT calculations using VASP code. In the DFT calculations, the wavefunctions of the relevant bands at the four time-reversal points in the form of plane waves (coefficient and wave vector) are stored in the WAVECAR file. The parity of a wavefunction can therefore be determined from these plane waves. The parity tables and the Z_2 topological invariant (v) for the SOC gap (Δ_1) between the top flat band and the top Dirac band and the SOC gap (Δ_2) between the two Dirac bands are listed in Table S1 and Table S2. It is clear that the two SOC gaps are topologically nontrivial.

It is noteworthy that the parities and δ_i values of the three M points are no longer equivalent. This is because the origin of the lattice was set to the center of a C-C bond The C6 symmetry no longer exits, leading to different parities of the three M points. If the origin is set to the center of the large hexagonal ring composing of six triazines, C6 symmetry is preserved and the three M points become equivalent. But the Z_2 topological invariant remains unchanged. Similar features have also been reported in a previous literature [2].

Table S1. The parity tables and the Z_2 topological invariant for the SOC gap (Δ_1)

Γ_i	Parity of ξ_{2n} of occupied bands	δ_i
(0, 0)	+ + - - + - - - - + - + - - - - - + - - + + - + - -	-
(1/2, 0)	- + - + - + - + - + + + + - + + - + - + + - + + - -	-
(0, 1/2)	- + - + - + - + - + + + + - + + - + - + + - + + - -	-
(1/2, 1/2)	- + + + - - + + - - - + - - + + + + - + + - - + + -	+
	Z_2 topological invariant	ν=1

Table S2. The parity tables and the Z_2 topological invariant for the SOC gap (Δ_2)

Γ_i	Parity of ξ_{2n} of occupied bands	δ_i
(0, 0)	+ + - - + - - - - + - + - - - - - + - - + + - + -	+
(1/2, 0)	- + - + - + - + - + + + + - + + - + - + + - + + -	+
(0, 1/2)	- + - + - + - + - + + + + - + + - + - + + - + + -	+
(1/2, 1/2)	- + + + - - + + - - - + - - + + + + - + + - - + +	-
	Z_2 topological invariant	ν=1

Part III. Phonon spectra of the g-$C_{12}N_6$ and g-$C_{24}N_6H_{12}$

We confirmed the kinetic stability of g-$C_{12}N_6$ and g-$C_{24}N_6H_{12}$ lattices using the same strategy as that of g-C_6N_6 lattice. The phonon dispersion relations along high-symmetric directions in BZ are plotted in Fig. S2. Clearly, both the phonon spectrums are free from imaginary frequencies, suggesting that all of them are kinetically stable.

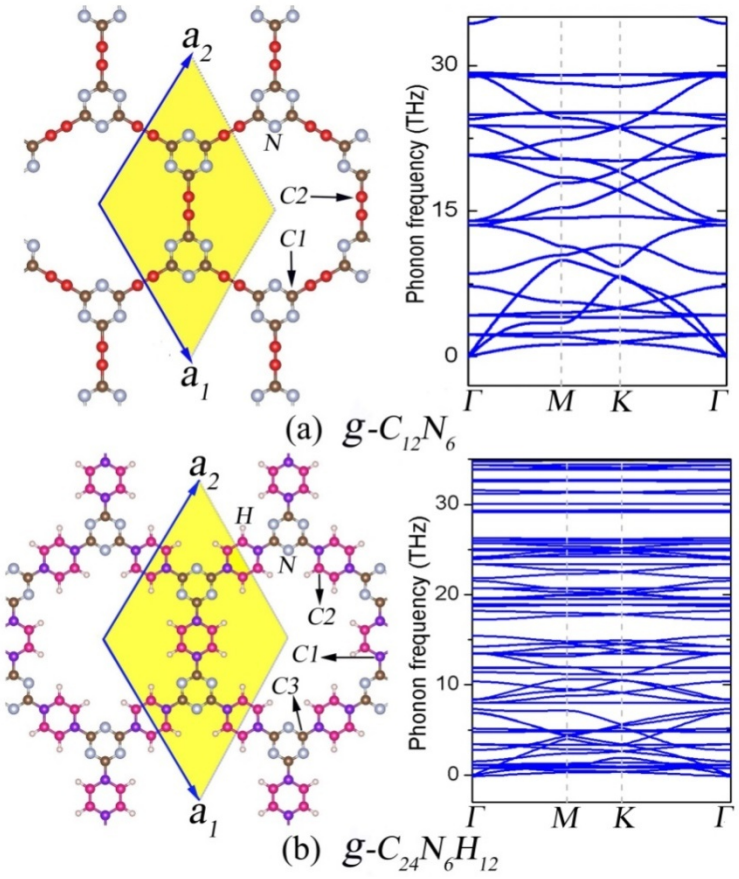

Fig. S2 Schematic representations of the honeycomb lattices of (a) g-$C_{12}N_6$ and (b) g-$C_{24}N_6H_{12}$. Unit cells are indicated by the yellow shaded area. The two basis vectors are represented by $\mathbf{a_1}$ and $\mathbf{a_2}$. Phonon spectrums along the high symmetric points in BZ are presented in corresponding right panel.

References

1. X. Hu, M. Kargarian and G. A. Fiete, *Phys. Rev. B*, 2011, **84**, 155166.
2. L. Fu and C. Kane, *Phys. Rev. B,* 2009, **79**, 161408.