We propose a class of nodal line semimetals that host an eight-fold degenerate double Dirac nodal line (DDNL) with negligible spin-orbit coupling. We find only 5 of the 230 space groups host the DDNL. The DDNL can be considered as a combination of two Dirac nodal lines, and has a trivial Berry phase. This leads to two possible but completely different surface states, namely, a torus surface state covering the whole surface Brillouin zone and no surface state at all. Based on first-principles calculations, we predict that the hydrogen storage material LiBH is an ideal DDNL semimetal, where the line resides at Fermi level, is relatively flat in energy, and exhibits a large linear energy range. Interestingly, both the two novel surface states of DDNL can be realized in LiBH. Further, we predict that with a magnetic field parallel to DDNL, the Landau levels of DDNL are doubly degenerate due to Kramers-like degeneracy and have a doubly degenerate zero-mode.

**Table I.** Space groups allowing for DDNL with negligible SOC effect.

| SG No. | BZ Location | 
|--------|-------------|
| 57     | \(\Gamma_0\) RT: \(\{\alpha, \frac{1}{2}, \frac{1}{2}\}\) |
| 60     | \(\Gamma_0\) RU: \(\{\frac{1}{2}, \alpha, \frac{1}{2}\}\) |
| 61     | \(\Gamma_0\) RT: \(\{\alpha, \frac{1}{2}, \frac{1}{2}\}\), RU: \(\{\frac{1}{2}, \alpha, \frac{1}{2}\}\), RS: \(\{\frac{1}{2}, \frac{1}{2}, \alpha\}\) |
| 62     | \(\Gamma_0\) RS: \(\{\frac{1}{2}, \frac{1}{2}, \alpha\}\) |
| 205    | \(\Gamma_c\) RM: \(\{\frac{1}{2}, \frac{1}{2}, \alpha\}\) |
find that only 5 SGs can exhibit the DDNL, which resides along the high-symmetry line located at the boundary of BZ. The five SGs and the location of DDNL in BZ are given in Table. 1. Particularly, for all the five SGs, the DDNL is the only possible degeneracy at the corresponding high-symmetry line(s), indicating that the number of the electronic bands of materials belonging to these SGs must be a multiple of 8 (including spin degree of freedom). Hence, for the material belonging to these SGs and having $8n + 4$ (with $n$ an integer) electrons, it must be a DDNL semimetal enforced by the filling [53].

The DDNL is topologically distinct from the usual Dirac nodal line (with $\pi$ Berry phase) in that its Berry phase is $2\pi$, as it can be considered as a combination of two Dirac nodal lines. Since the Berry phase is defined mod of $2\pi$, it is trivial for DDNL. As a consequence, the DDNL features two distinct states at the boundary of system, as schematically shown in Fig. 1(c–d), which both are completely different from the drumhead-like surface state in usual NL [see Fig. 1(a–b)]. One is the novel surface state spanning over the whole surface BZ [see Fig. 1(c)]. Since the 2D surface BZ is a torus, such novel surface state then is termed as torus surface state [39, 54]. The other case is that no surface state appears on the surface, even though there exists an NL (e.g. DDNL) in bulk [see Fig. 1(d)]. These two cases are topologically allowed and consistent with the trivial Berry phase of DDNL. Moreover, we predict that by applying a magnetic field parallel to the line, the Landau levels of DDNL are doubly degenerate due to Kramers-like degeneracy and have a doubly degenerate zero-mode, which shall suggest pronounced signature in magneto-transport.

We demonstrate our ideas by the first-principles calculations and model analysis of a concrete material. We find the hydrogen storage material LiBH is an ideal DDNL semimetal candidate, where the DDNL resides at Fermi level, is relatively flat in energy, and exhibits a large linear energy range. Interestingly, both torus surface state and no surface state simultaneously appear in LiBH material. More importantly, we calculate the LL spectrum of a lattice model based on LiBH and find the doubly degenerate zero-mode LL can be clearly observed. These results indicate that the novel properties of DDNL predicted here should be experimentally detected in LiBH. Thus, our work not only predicts a new semimetal phase, but also shows an ideal material platform for exploring interesting fundamental physics connected to it.

**Crystalline structure and electronic bands.** We motivate our investigation by considering the hydrogen storage material LiBH [55]. This material has a orthorhombic structure with SG Pnma (No. 62), which is one candidate in Table I. The primitive cell of LiBH contains in total 12 atoms with Li, B and H residing at the 4c Wyckoff positions, as shown in Fig. 2(a). Since all the three atoms: Li, B and H are lighter than carbon, the SOC effect in LiBH is negligibly small, and we virtually obtain a spinless system. This is a precondition for realizing DDNL, as the DDNL is not robust against SOC [52]. Moreover, the electron number of LiBH is 20 ($= 2\times 8 + 4$). Therefore, the LiBH material is a filling-enforced DDNL semimetal with the line appearing around Fermi level. The lattice constants obtained from our first-principles calculations are $a = 6.2$ Å, $b = 3.0$ Å and $c = 6.3$ Å [56], consistent with previous result [55]. The symmetry operators of SG 62 are generated by two screw rotations $\bar{C}_{2z} = \{C_{2z}|\frac{1}{2}0\frac{1}{2}\}$ and $\bar{C}_{2y} = \{C_{2y}|0\frac{1}{2}0\}$, and a spatial inversion $P$. The material also has time-reversal symmetry $T$ with $T^2 = 1$, corresponding to the negligible SOC effect in LiBH.

The calculated electronic band structure of LiBH without SOC is presented in Fig. 3(a). It is clearly shown that this material is a DDNL semimetal with the line appearing at RS path, consistent with symmetry analysis (see Table I). A remarkable feature of the electronic bands of LiBH is that its low-energy spectra is roughly symmetric about Fermi level, indicating that LiBH has an approximate chiral symmetry [57]. From Fig. 3(a), one observes that there exist two band crossings almost cutting the Fermi level. We first consider the linear crossing (labelled as A) on FY path. Due to the presence of $\bar{M}_{z} = \bar{C}_{2z}P$ and $PT$ symmetry, point A can not appear
The algebra satisfied by the three generators at $D$ on RS passing through hourglass NL. Thus, they can be expressed as

$$\hat{C}_{2z} = \sigma_0 \otimes \sigma_z, \quad \hat{M}_y = \sigma_z \otimes \sigma_x, \quad A = i\sigma_y \otimes \sigma_0 \mathcal{K},$$

with $\mathcal{K}$ the complex conjugation. With the standard approach \[19, 60\], the effective $k$-$p$ Hamiltonian for a generic point on DDNL can be obtained as

$$\mathcal{H}_{\text{DDNL}} = \left( c_1 + c_2 k_z \right) + \begin{bmatrix} h_D & h' \\ h'^\dagger & h_D \end{bmatrix},$$

with $h_D = \alpha k_x \sigma_x + \beta k_y \sigma_y$ and $h' = \alpha k_z \sigma_z + \beta k_y \sigma_x$. Here, $c_1, c_2, \alpha, \beta$ are real parameters, and $\alpha$ and $\beta$ are complex parameters. Clearly, the obtained Hamiltonian (5) is consistent with Eq. (1) in Introduction, which directly demonstrates the existence of DDNL in LiBH. Due to nonvanishing off-diagonal terms $h'$, the two Dirac cones described by $h_D$ would split at a general momentum point, while are stucked together along $k_{x(\parallel)} = 0$ axis [see Fig. 3(c)], resulting from the nodal surfaces on boundaries.

**Torus surface state.** We then explore the surface state of LiBH. It is has been extensively shown that NL semimetals feature drumhead-like surface state at sample boundary, due to $\pi$ Berry phase of the line. This is the case for the hourglass NL in LiBH, which has $\pi$ Berry phase and leads a drumhead-like surface state at (001) surface, as shown in Fig. 4(c,f). However, both (100) and (010) surfaces, which are parallel to DDNL, do not exhibit drumhead-like surface state. More surprisingly, the (100) surface has a torus surface state covering the whole (100) surface BZ, as shown in Fig. 4(a,d), and in sharp contrast, the (010) surface does not have any surface state [Fig. 4(b,e)].

The surface state in NL semimetal generally is protected by quantized $\pi$ Zak phase, which is the Berry phase of a straight line normal to the surface and crossing the bulk BZ \[61\]. Here, due to the presence of $\mathcal{P}$ symmetry in LiBH, the Zak phase is quantized to be $0$ or $\pi$, corresponding two topologically distinct phases.

We first study the surface state on (100) surface. Starting from the Zak phase $\mathcal{Z}(k_y = 0, k_z)$ (with $k_z \neq 0$) of...
FIG. 4. (a-c) Schematic figures of the surface state for (100), (010) and (001) surfaces. The values 0 and ±\(\pi\) in (a-c) are the Zak phase for lines normal to the corresponding surface. (d-f) Surface spectra on (100), (010) and (001) surfaces. In (d), the surface state spans the whole surface BZ, leading to the torus surface state, while in (e) no surface state can be observed.

DDNL also has a zero-mode LL for each \(k_z\)-fixed plane [56], as shown in Fig. 5(a,b). Moreover, these zero-mode LLs are doubly degenerate. While the \(B\) field breaks both \(T\) and \(C_{2y}\) symmetries, it preserves \(A = (C_{2y} T)\) symmetry, and then all the LL bands (including zero-mode LLs) of DDNL are doubly degenerate resulting from the Kramers-like degeneracy produced by \(A^2 = -1\). Since the degeneracy of the two zero-mode LLs is protected by \(A\) symmetry, it would be robust against \(B\) field and always exist regardless of the filed strength. Given the fact that the zero-mode LL in graphene gives rise to many novel phenomena [64], one can expect the DDNL may exhibit interesting magnetoresponses distinct from the usual Dirac NLs and also 2D Dirac semimetal.

Particularly, the low-energy spectrum of LiBH is so clean that the LL properties proposed here shall be observed in it. We further demonstrate it by calculating the LL spectrum of a lattice model based on LiBH material. The calculated results are given in Fig. 5(c), where a doubly degenerate LL with almost flat dispersion occurring at the Fermi level, corresponding to the doubly degenerate zero-mode LL. This strongly suggests that the unusual LL spectrum of DDNL can be detected in LiBH by magnetotransport measurements.

**Conclusion.** In summary, we propose a new class of semimetal phase: DDNL in LiBH material. The DDNL can be considered as a combination of two Dirac NLs and exhibits many distinct phenomena, such as torus surface state and unusual LL spectrum. In particular, we predict LiBH material is an ideal DDNL semimetal and demonstrate that the novel phenomena of DDNL predicted here can be clearly observed in LiBH material. Moreover, as the torus surface in LiBH is rather flat in energy [see Fig. 4(a)], it will be interesting to explore possible unconventional superconductivity, correlation effect and magnetism in LiBH (100) surface.

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See Supplemental Material for the computational methods, the tight-binding model, and the Landau levels.

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