Supplementary information to "Statistical learning of engineered topological phases in the kagome superlattice of AV_3Sb_5"

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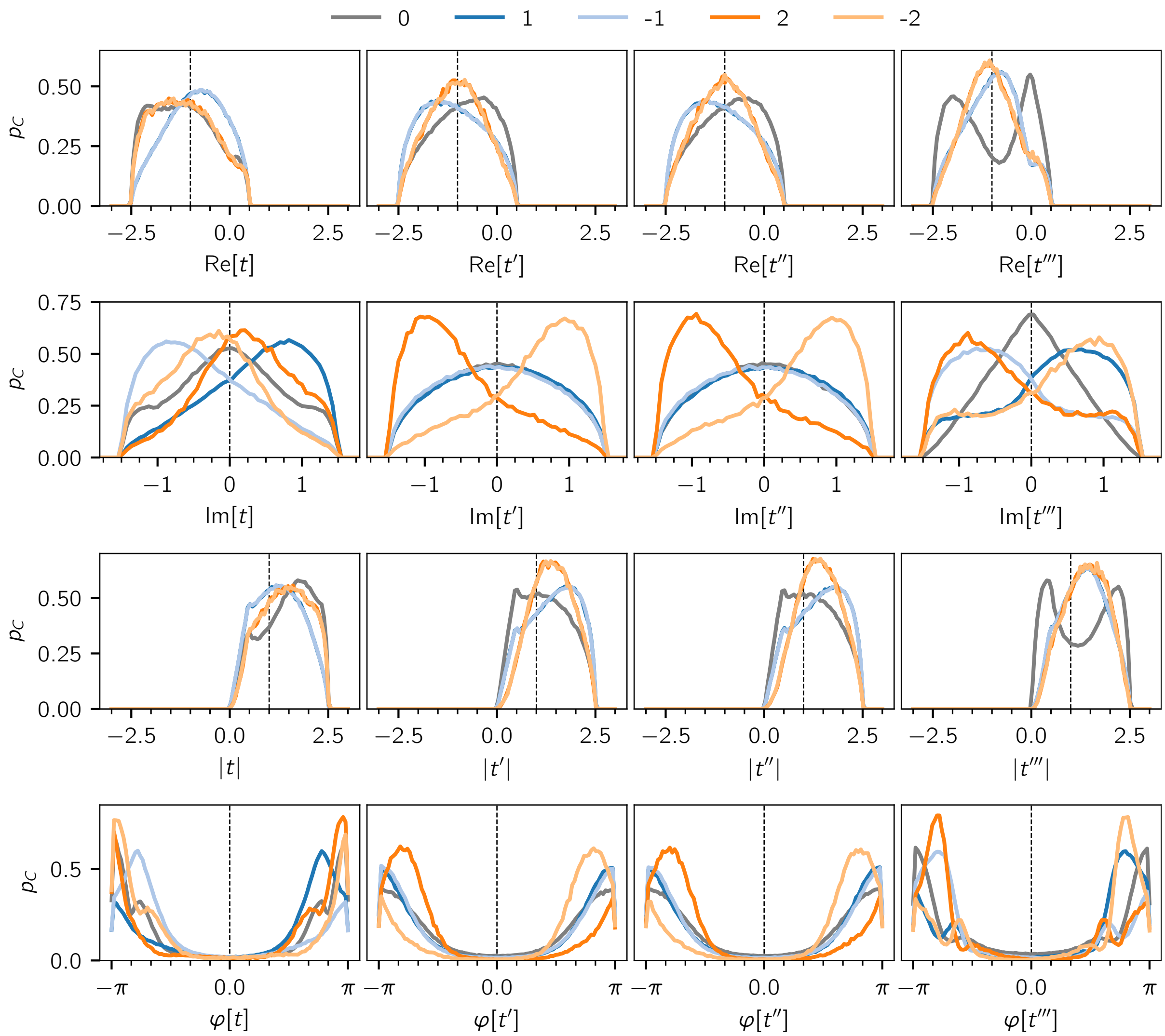
Supplementary Fig. 1 shows the marginal probability distribution functions (PDFs) for all the hoppings $[t, t', t'', t''']$ for insulators within the 2×2 kagome superlattice with C_6 symmetry, with the corresponding Chern label as indicated by the color legend on top. The vertical dashed lines mark the reference point for the initial configuration, around which the randomized data-sets were generated from a uniform distribution function. The top row shows the PDF of the $\mathrm{Re}[\cdot]$ component of the hopping distributions, the rows below contain its imaginary components $\mathrm{Im}[\cdot]$, the modulus $|\cdot|$ and the argument $\varphi[\cdot]$ of the individual hopping terms (in this order). As mentioned earlier in the main text, we notice that the PDF for t' and t'' are the same due to the inherent symmetry of the lattice, hence we will focus our discussion on the PDF of t' only. Observing the PDFs, one can gain insight into the bond strength and the direction of the complex hoppings (windings) by investigating the modulus $|\cdot|$ and $\mathrm{Im}[\cdot]$ of the hoppings, respectively. These two features encode the complete description of the real-space manifestation of the topological properties that we focused on in our analysis.

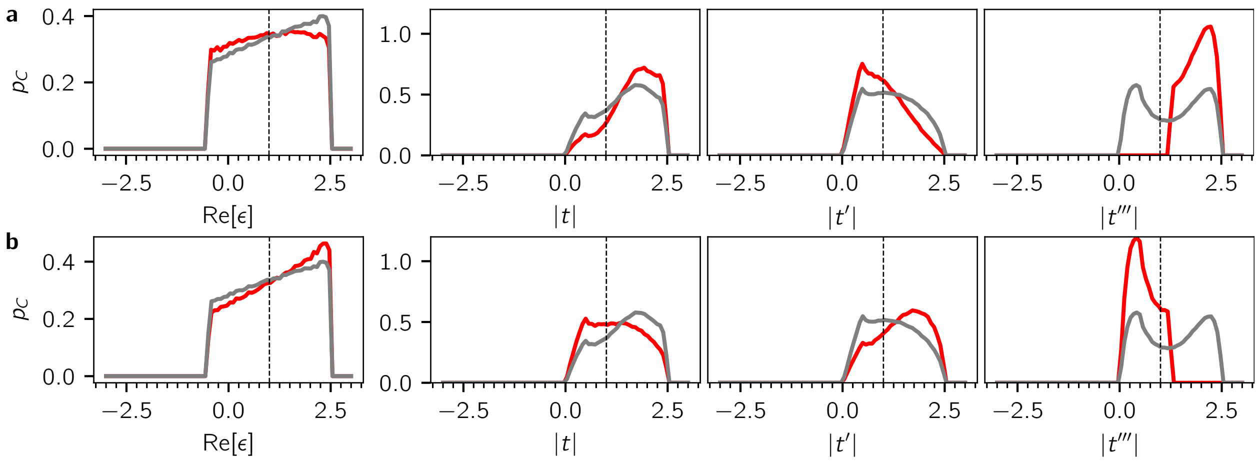
We interpret the positive values of the $\mathrm{Im}[\cdot]$ PDFs to be aligned in the direction of the original hoppings of our tight-binding Hamiltonian (as shown in Fig. 2b in the main text), and the negative values of $\mathrm{Im}[\cdot]$ PDFs denote hoppings in the opposite direction w.r.t the original convention. Following this, we conclude that the trivial $C = 0$ phase PDFs $p_0(\mathrm{Im}[t])$, $p_0(\mathrm{Im}[t'])$ and $p_0(\mathrm{Im}[t'''])$ (Fig. 1) show a maximum at zero and perfectly symmetric behavior around it. Hence, no particular hopping direction is preferred. However, the non-trivial $C = +1$ phase PDFs, $p_1(\mathrm{Im}[t])$ and $p_1(\mathrm{Im}[t'''])$, show maxima for positive $\mathrm{Im}[t]$ and $\mathrm{Im}[t''']$, while the maxima for the $C = -1$ phase lie in the opposite half of the distribution. This preferred direction of the hopping is illustrated in the phase diagram in Fig. 4 of the main text as the clockwise or anticlockwise winding of the flux patterns for the $C = \pm 1$ phase. Since $p_{\pm 1}(\mathrm{Im}[t'])$ is symmetric around its maximum at zero, we conclude that t' has no preferred direction of orientation to distinguish the $C = \pm 1$ Chern phase from $C = 0$. Next, we applied a similar approach of our analysis to the PDFs of $p_C(\mathrm{Im}[t])$, $p_C(\mathrm{Im}[t'])$ and $p_C(\mathrm{Im}[t'''])$ for the $C = \pm 2$ phase and arrived at the conclusions presented in the main text.

In the following, we describe our approach to analyze the moduli $|\cdot|$ of the individual hopping terms to characterize bond strength signatures corresponding to the trivial phase. First, we pick the most prominent feature for the trivial $C = 0$ phase, as seen in the PDF $p_0(|t'''|)$, that shows a double-dome structure with two local maxima of similar magnitude. By restricting the data set to the samples with $|t'''| > 1.25$, we find the constrained PDFs as shown in Fig. 2(a) below. The black lines denote the full PDFs and the red lines denote the PDFs of the restricted data set with $|t'''| > 1.25$. For this strong bond strength $|t'''|$ relative to the reference point [depicted in red for $p_0(|t'''|)$] we find that $p_0(|t|)$ also displays a maximum at $|t|$ larger than its reference value. The distribution $p_0(|t'|)$, however, shows maxima below the reference point in this case, suggesting a relatively weaker bond strength of $|t'|$. This bond strength configuration is the *inverse* Star-of-David-like charge bond order pattern that we referred to in the main text. In Fig. 2(b) we plot the PDFs for the restricted data set for the samples that lie on the other side of the dome, i.e., $|t'''| < 1.25$, in red. Here, we find that the maxima of $p_0(|t'''|)$ and $p_0(|t|)$ both are below the reference value (relatively weaker bond strength) while that of $p_0(|t'|)$ is above the reference value (relatively stronger bond strength). This bond strength pattern is the Star-of-David-like charge bond order pattern.

The behavior of $|t|$ aligns with the trend of $|t'''|$, and hence, we arrive at the conclusion of the possible Star-of-David or inverse Star-of-David-like bond strength patterns as a characteristic signature of the trivial phase ($C = 0$). The PDFs of $|\cdot|$ in the non-trivial phases ($C \neq 0$) do not have a prominent distinguishing behavior or structure like the trivial phase, and display very similar bond strength across all hoppings. Thus, a further analysis on them was not carried out.



Supplementary Figure 1. **Marginal probability distributions.** Marginal PDFs for real part Re[$\cdot$], imaginary part Im[$\cdot$], phase $\varphi[\cdot]$ and modulus $|\cdot|$ of all hoppings for insulators within the 2×2 kagome superlattice with C_6 symmetry. Gray lines denote trivial phases ($C = 0$) and colored lines denote non-trivial ($C \neq 0$) phases as given by the legend on top. The reference point is indicated by dashed vertical lines.



Supplementary Figure 2. **Marginal probability distributions for trivial insulators.** Marginal PDFs for the real onsite term and moduli of the hoppings for trivial insulators ($C = 0$) within the 2×2 kagome superlattice with C_6 symmetry are shown in gray. With red lines, we show the marginal PDFs for a restricted data set, where (a) $|t'''| > 1.25$ yielding an inverse Star of David pattern, and (b) $|t'''| < 1.25$ yielding a Star of David pattern. The reference point is indicated by dashed vertical lines.