

# Intertwined Van Hove Singularities as a Mechanism for Loop Current Order in Kagome Metals

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Recent experiments on kagome metals  $AV_3Sb_5$  ( $A = Cs, Rb, K$ ) indicated spontaneous time-reversal symmetry breaking in the charge density wave state in the absence of static magnetization. The loop current order (LCO) is proposed as its cause, but a microscopic model explaining the emergence of LCO through electronic correlations has not been firmly established. We show that the coupling between van Hove singularities with distinct mirror symmetries is a key ingredient to generate LCO ground state. By constructing an effective model, we find that when multiple van Hove singularities with opposite mirror eigenvalues are close in energy, the nearest-neighbor electron repulsion favors a ground state with coexisting LCO and charge bond order. It is then demonstrated that this mechanism applies to the kagome metals  $AV_3Sb_5$ . Our findings provide an intriguing mechanism of LCO and pave the way for a deeper understanding of complex quantum phenomena in kagome systems.

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**Introduction.**—The vanadium-based kagome metals  $AV_3Sb_5$  ( $A = Cs, Rb, K$ ) have generated considerable interest due to the discovery of exotic phases in this family of materials [1–28]. Superconductivity in these materials emerges at  $T_c \sim 0.9$ – $2.8$  K [29–32], with magnetoresistance measurements indicating the possibility of novel superconductivity with charge  $4e$  and  $6e$  flux quantization [33]. Additionally, a  $2 \times 2$  charge density wave (CDW) is detected below  $T_{CDW} \sim 80$ – $100$  K [29,34–38] with scanning tunneling microscopy, emphasizing the important role of van Hove singularities (vHSs) at  $M$  point of the Brillouin zone. Intriguingly, these materials exhibit spontaneous time-reversal symmetry breaking after the CDW transition, evidenced through techniques such as muon spin relaxation and scanning tunneling microscope [12,35,39] in the CDW phase without evidence of static magnetic order [30,34,40]. These observations indicate an unconventional CDW order in  $AV_3Sb_5$ .

The observation of time-reversal symmetry breaking without static magnetic order leads to the hypothesis of loop current order (LCO) [12,41–43], but the mechanism to generate LCO remains unclear. Enormous experimental and theoretical efforts are devoted to determine the properties of CDW in this kagome system [9,13,20,36,42–72]. The simplest way to model the system is through a three-band model obtained by assigning a single orbital to each site. When the chemical potential is close to the vHS, incorporating nearest neighbor (NN) electron interactions and electron-phonon coupling leads to a charge bond order (CBO) ground state rather than LCO [20]. Reference [43] shows that LCO can be induced by electron interaction, but this necessitates a substantial next-nearest-neighbor

interaction, a condition not aligned with realistic scenarios. This poses a critical question: what are the conditions for the emergence of LCO in generic kagome materials?

Noticing the presence of multiple vHSs in  $AV_3Sb_5$ , in this Letter we demonstrate that when two vHSs with *different mirror symmetry eigenvalues* are close to the Fermi level, a simple NN interaction can generate LCO when the coupling between different vHSs is taken into account. This ground state has LCO coexisting with CBO, dubbed loop current charge bond order (LCBO). We apply this analysis to  $AV_3Sb_5$  by considering a tight binding model with multiple vHSs. We find that the ground state of  $AV_3Sb_5$  is LCBO under the conditions described below. This study unveils a mechanism for generating LCO in kagome systems with multiple vHSs.

**Conditions imposed by mirror symmetries.**—We first show that mirror symmetries impose important constraints on the wave functions at vHSs, which are key ingredients for the emergence of LCBO. Each vHS at momentum  $M$  has little group  $D_{2h}$  with mutually perpendicular mirror planes  $m_z, m', m''$ , where  $m_z$  coincides with kagome plane,  $m'$  and  $m''$  are shown in Fig. 1(a). Consider two vHSs near the Fermi level denoted by VH1 and VH2 at the three distinct momenta  $M$  denoted by  $M_A, M_B, M_C$  as in Fig. 1(a). We show that mirror symmetries will constrain the wave function of VH1 and VH2 at three distinct  $M$  points to take the form of Fig. 1(c) as long as the following conditions are satisfied: (1) the wave functions of VH1 and VH2 have opposite eigenvalues under  $m'$  and the same eigenvalues under  $m''$ , and (2) VH1 and VH2 consist of the same type of orbital at the kagome sites.

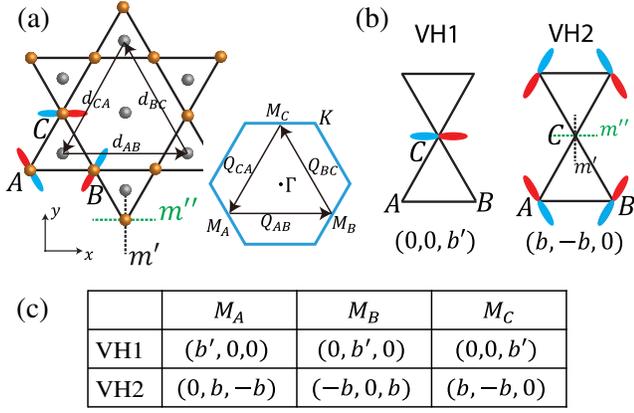


FIG. 1. (a) Kagome plane of  $AV_3Sb_5$  ( $A = Cs, Rb, K$ ). The red (blue) parts denote regions of orbitals with positive (negative) amplitude. The inset shows the Brillouin zone. (b) Real space wave function of VH1 and VH2 at  $M_C$  allowed by mirror symmetries. (c) Weight of wave function in  $(A, B, C)$  sublattices for VH1 and VH2 at three distinct  $M$  points imposed by mirror symmetries, where  $b$  and  $b'$  are constants.

To demonstrate this conclusion explicitly, we consider two vHSs made of the colored orbitals in Fig. 1(a), and let the wave function at VH1 (VH2) be odd (even) under  $m'$ . Let us inspect the form of symmetry-allowed wave function at momentum  $M_C$  as shown in Fig. 1(b). In this case,  $m'$  coincides with  $m_x$ , which maps sublattice  $A$  and  $B$  to each other and maps sublattice  $C$  to itself. Because the wave function of VH2 is even under  $m'$  and the orbital at sublattice  $C$  is odd under  $m'$ , the weight of wave function must vanish at  $m'$ -invariant sublattice  $C$ . Furthermore, wave function components of VH2 at sublattice  $A$  and  $B$  must have opposite signs to make the wave function even under  $m'$ . Therefore, the wave function of VH2 at momentum  $M_C$  must take the form  $(b, -b, 0)$  at  $A, B, C$  sublattices respectively, where  $b$  is a constant. A similar analysis can be applied to VH1, which gives the form of  $(0, 0, b')$  instead, where  $b'$  is another constant. Finally, the threefold rotation symmetry leads to the wave function structure at the three distinct  $M$  points given in Fig. 1(c). Similarly, this wave function structure can also be obtained for orbitals with other mirror eigenvalues, as shown in Sec. I of the Supplemental Material (SM) [73].

*Effective model for coupled vHSs.*—We construct an effective model that describes the coupling between different vHSs. The order parameter for a complex CDW with  $2 \times 2$  periodicity is written as

$$\Delta_{\alpha\beta} = \frac{V}{2N_c} \sum_{\mathbf{R}} (\langle c_{\mathbf{R},\alpha}^\dagger c_{\mathbf{R},\beta} \rangle - \langle c_{\mathbf{R},\alpha}^\dagger c_{\mathbf{R}-\mathbf{d}_{\alpha\beta},\beta} \rangle) \cos(\mathbf{Q}_{\alpha\beta} \cdot \mathbf{R}). \quad (1)$$

Here,  $\mathbf{R}$  labels unit cells,  $V$  is the NN interaction strength,  $N_c$  is the number of unit cells,  $\alpha, \beta = A, B, C$  denote the

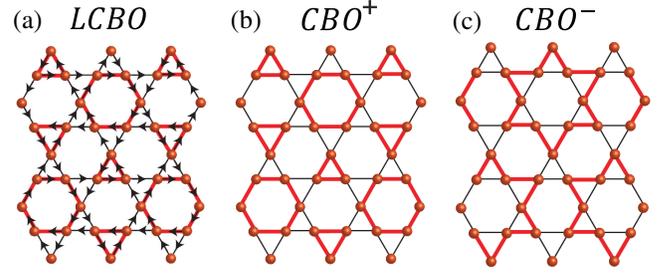


FIG. 2. (a) Coexisting loop current order and charge bond order (LCBO). The red bonds represent modulations of  $\langle c_{\mathbf{r}}^\dagger c_{\mathbf{r}'} \rangle$  at NN bonds and the arrows represent current  $I \sim \langle ic_{\mathbf{r}}^\dagger c_{\mathbf{r}'} - ic_{\mathbf{r}'}^\dagger c_{\mathbf{r}} \rangle$ . (b) Charge bond order with  $\Delta > 0$ . (c) Charge bond order with  $\Delta < 0$ .

kagome sublattices, and  $\mathbf{Q}_{\alpha\beta}$  connects different momenta  $M$  as in Fig. 1(a). In phases that preserve threefold rotation symmetry, the order parameters satisfy  $\Delta_{AB} = \Delta_{BC} = \Delta_{CA} \equiv \Delta$ . The real part of  $\Delta$  represents CBO, the imaginary part represents LCO, and a complex value of  $\Delta$  represents the coexisting phase of LCO and CBO, denoted as LCBO in Fig. 2(a). The phase with real  $\Delta > 0$  ( $\Delta < 0$ ) is denoted as  $CBO^+$  ( $CBO^-$ ) as shown in Figs. 2(b) and 2(c). There are other possible LCO phases distinct from the ones in Fig. 2, but those phases have higher free energy as shown in Sec. IV of SM; hence, we mainly focus on the phases in Fig. 2.

We can construct an effective model on patches near the three  $M$  points. This model can effectively capture the coupling between different vHSs, which is the dominant contribution leading to the LCBO ground state. The coupling between vHSs at different  $M$  points is proportional to the order parameter with coupling strength determined by the wave function components at vHSs. We choose the basis  $u_1(M_A), u_1(M_B), u_1(M_C), u_2(M_A), u_2(M_B), u_2(M_C)$  where  $u_1, u_2$  denotes the wave function for VH1 and VH2 respectively. Let  $\mathbf{k}$  denote the small deviation from  $M$  with  $|\mathbf{k}| < k_{\text{cut}}$ . Given the form of wave functions in Fig. 1(c) and the order parameter in Eq. (1), the effective Hamiltonian with leading terms in  $\mathbf{k}$  is derived in Sec. II of SM to be

$$H_{\text{eff}}(\mathbf{k}, \Delta) = \begin{pmatrix} \epsilon_1 & s_1 \Delta & s_1 \Delta^* & \lambda^* k_1 & 0 & 0 \\ s_1 \Delta^* & \epsilon_1 & s_1 \Delta & 0 & \lambda^* k_2 & 0 \\ s_1 \Delta & s_1 \Delta^* & \epsilon_1 & 0 & 0 & \lambda^* k_3 \\ \lambda k_1 & 0 & 0 & \epsilon_2 & s_2 \Delta^* & s_2 \Delta \\ 0 & \lambda k_2 & 0 & s_2 \Delta & \epsilon_2 & s_2 \Delta^* \\ 0 & 0 & \lambda k_3 & s_2 \Delta^* & s_2 \Delta & \epsilon_2 \end{pmatrix}, \quad (2)$$

$$\equiv \begin{pmatrix} P_1 & Q^\dagger \\ Q & P_2 \end{pmatrix}.$$

Here,  $P_1, P_2, Q$  are  $3 \times 3$  matrices,  $k_1 = -\frac{1}{2}k_x + (\sqrt{3}/2)k_y$ ,  $k_2 = -\frac{1}{2}k_x - (\sqrt{3}/2)k_y$ ,  $k_3 = k_x$ .  $\epsilon_1$  and  $\epsilon_2$  denote the

energies of VH1 and VH2, respectively. The chemical potential  $\mu$  is set between  $\epsilon_1$  and  $\epsilon_2$ . Let us first inspect the form of  $P$  matrices imposed by symmetries. The matrix  $P_1$  ( $P_2$ ) describes the effect of CDW order on VH1 (VH2) at momenta  $M_A$ ,  $M_B$ ,  $M_C$ . The threefold rotation symmetry permutes the three  $M$  points, which requires  $(P_n)_{12} = (P_n)_{23} = (P_n)_{31}$  for  $n = 1, 2$ , and whether these matrix elements are related to  $\Delta$  or  $\Delta^*$  is determined by the wave function at the vHS. The coefficients  $s_1$  and  $s_2$  are determined by wave functions at the vHS, which are found to be  $s_1 = -2|b'|^2$  and  $s_2 = 2|b|^2$ . The relative sign difference in these coefficients comes from the  $-b$  term in Fig. 1(c) as shown in Sec. III of SM, which is a consequence of the mirror symmetries.

Another important consequence of the mirror symmetries is that they enforce the  $Q$  matrix in the off-diagonal block to be a diagonal matrix. With the wave function structure in Fig. 1(c), the off-diagonal elements of  $Q$  must vanish because they are multiplied by the zeros of wave function components from either VH1 or VH2, as shown in Sec. III of SM. Therefore, only the diagonal terms remain in the  $Q$  matrix, which describes the coupling between two vHSs at the same  $M$  point. These terms are linear in  $\mathbf{k}$  because  $\epsilon_1$  and  $\epsilon_2$  are exact eigenvalues when both  $\mathbf{k}$  and  $\Delta$  are zero; hence, at  $\mathbf{k} = 0$  the diagonal terms should vanish and the leading order is linear in  $\mathbf{k}$ .

*Mechanism to generate LCBO.*—We now discuss the last condition for LCBO to be the ground state of a system described by Eq. (2). To derive this, we start from the limit with  $\lambda = 0$  and do a perturbation theory on  $\lambda$ . When  $\lambda = 0$ ,  $H_{\text{eff}}(\mathbf{k}, \Delta)$ , and  $H_{\text{eff}}(\mathbf{k}, \Delta e^{(2\pi i/3)})$  have the same eigenvalues because they are related by a gauge transformation  $\mathcal{U} = \text{diag}\{1, \omega, \omega^*, 1, \omega^*, \omega\}$  with  $\omega = e^{(2\pi i/3)}$ . Hence, when  $\lambda = 0$  the free energy  $F$  is invariant under  $\Delta \rightarrow \Delta e^{(2\pi i/3)i}$ , and  $F$  has degenerate minima at  $\Delta = -|\Delta|$  and  $\Delta = |\Delta|e^{\pm(\pi/3)i}$  corresponding to CBO<sup>-</sup> and LCBO respectively. The eigenvalues of  $H_{\text{eff}} - \mu$  at both minima are the same, which are given by

$$\begin{aligned} E_1 = \epsilon_2 - \mu - 4|b|^2|\Delta|, \quad E_2 = E_3 = \epsilon_1 - \mu - 2|b'|^2|\Delta|, \\ E_4 = E_5 = \epsilon_2 - \mu + 2|b|^2|\Delta|, \quad E_6 = \epsilon_1 - \mu + 4|b'|^2|\Delta|. \end{aligned} \quad (3)$$

When the energy separation between VH1 and VH2 is small, the sign of each eigenvalue is determined by the  $\Delta$  term; hence, the negative eigenvalues are  $E_1, E_2, E_3$ . In the low-temperature limit the sum of them determines the free energy. When  $\lambda$  becomes finite, the degenerate minima of  $F$  at  $\Delta = -|\Delta|$  and  $|\Delta|e^{\pm(\pi/3)i}$ , corresponding to CBO<sup>-</sup> and LCBO splits. The amount of splitting can be computed by degenerate perturbation theory that captures the evolution of  $E_{1-3}$  with  $\lambda$ . Define  $\delta\epsilon \equiv \epsilon_2 - \epsilon_1$  as the separation between VH1 and VH2 and denote  $A$  as the system area. We find that the difference in free energy density  $f = F/A$  between CBO<sup>-</sup> and LCBO is given by

$$\begin{aligned} f_{\text{CBO}^-} - f_{\text{LCBO}} &= \sum_{|\mathbf{k}| \lesssim k_{\text{cut}}} \frac{-2|\lambda|^2(k_1k_2 + k_2k_3 + k_1k_3)|\Delta|(|b|^2 + |b'|^2)}{A(2|\Delta|(|b|^2 + |b'|^2) + \delta\epsilon)(4|\Delta|(|b|^2 + |b'|^2) - \delta\epsilon)} \\ &= \frac{3}{16\pi} \frac{|\lambda|^2 k_{\text{cut}}^4 |\Delta| (|b|^2 + |b'|^2)}{(2|\Delta|(|b|^2 + |b'|^2) + \delta\epsilon)(4|\Delta|(|b|^2 + |b'|^2) - \delta\epsilon)} > 0. \end{aligned} \quad (4)$$

Equation (4) shows that for small energy separation  $\delta\epsilon < 4(|b|^2 + |b'|^2)|\Delta|$ , a finite coupling  $\lambda$  between the two vHSs will make LCBO have lower energy and be more favorable than the competing phase CBO<sup>-</sup>. This is the mechanism to generate LCBO in kagome systems.

Importantly, we find that the LCBO phase cannot be described by a small order parameter expansion of the Ginzburg-Landau theory; hence, it is not sensitive to the dispersion near vHSs. In Sec. V of SM, we demonstrate that the solution corresponding to LCBO cannot be obtained from Ginzburg-Landau free energy even if high power terms of  $\Delta$  are included. We also reiterate that the free energy analysis in Eq. (4) leading to an LCBO ground state is a result of the coupling between two vHSs with distinct mirror symmetries.

*Application to AV<sub>3</sub>Sb<sub>5</sub>.*—We apply the above analysis to AV<sub>3</sub>Sb<sub>5</sub> and explicitly construct the effective Hamiltonian  $H_{\text{eff}}$ . We start from a tight binding model that captures multiple vHSs near the Fermi level. The bands close to the Fermi level in AV<sub>3</sub>Sb<sub>5</sub> are mainly made of  $d$  orbitals at  $V$  sites and  $p$  orbitals at Sb sites. We consider the tight binding model introduced in Ref. [68]. This model includes three  $p$  orbitals at each out-of-plane Sb site and one  $d$  orbital at each  $V$  site. This  $d$  orbital is made of a specific linear combination of  $d_{xz}, d_{yz}$  orbitals as indicated by the colored orbitals in Fig. 1(a), which is odd (even) under  $m'$  ( $m''$ ), denoted as  $\tilde{d}$  orbitals. Hence, there are three  $\tilde{d}$  orbitals and six  $p$  orbitals in each unit cell, leading to a nine-band model  $H_{\text{TB}}(\mathbf{k})$ . The hopping parameters in this model are obtained from density-functional theory (DFT) band structure [68]. The band structure of  $H_{\text{TB}}(\mathbf{k})$  is shown in Fig. 3(a). Compared with the DFT band structure in Fig. 3(b), the nine-band model reproduces two vHSs at momentum  $M$  denoted by VH1 and VH2. VH1 is odd (even) under  $m'$  ( $m''$ ) and is mainly made of  $\tilde{d}$  orbitals. VH2 is even under both  $m'$  and  $m''$  and is a superposition of  $\tilde{d}$  and  $p$  orbitals. Compared with commonly used three-band models that can only describe VH1, this nine-band model can capture both VH1 and VH2; hence, it provides a useful platform to study the interplay between different vHSs.

Next we consider the NN electron interaction given by

$$H_V = V \sum_{(\mathbf{R}\alpha; \mathbf{R}'\beta)} c_{\mathbf{R},\alpha}^\dagger c_{\mathbf{R},\alpha} c_{\mathbf{R}',\beta}^\dagger c_{\mathbf{R}',\beta}, \quad (5)$$

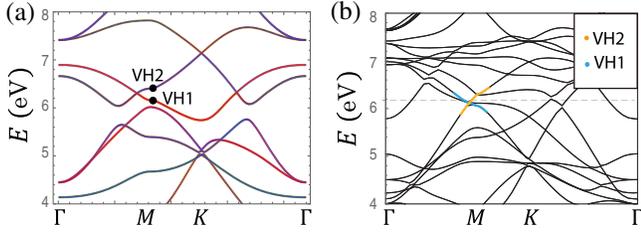


FIG. 3. (a) Band structure of the  $9 \times 9$  tight binding model  $H_{\text{TB}}(\mathbf{k})$  that can reproduce VH1 and VH2. The red color represents the weight of  $\tilde{d}$  orbitals in the wave function. (b) Band structure obtained from DFT with VH1 and VH2 highlighted. The figure is adapted from Ref. [68].

where  $\langle \mathbf{R}\alpha; \mathbf{R}'\beta \rangle$  denotes NN bonds. With the order parameter  $\Delta_{\alpha\beta}$  defined in Eq. (1), the NN interaction can be mean-field decoupled as [68]

$$H_V^{\text{MF}} = - \sum_{\mathbf{k}} (\Delta_{\alpha\beta} (1 - e^{i\mathbf{k} \cdot \mathbf{d}_{\alpha\beta}}) c_{\mathbf{k}-\mathbf{Q}_{\alpha\beta}, \beta}^\dagger c_{\mathbf{k}, \alpha} + \text{H.c.}) + 2N_c \frac{|\Delta_{\alpha\beta}|^2}{V}, \quad (6)$$

We can write down a mean-field Hamiltonian that includes all bands in Fig. 3(a) and the CDW order parameter in Eq. (6) with  $\Delta_{AB} = \Delta_{BC} = \Delta_{CA} \equiv \Delta$ . To construct the effective patch model  $H_{\text{eff}}$ , we focus on momenta near the  $M$  points and perform a unitary transformation into the band basis in which the basis functions at  $M$  points are eigenfunctions of the tight binding model. Then we keep only the matrix elements corresponding to the energies and couplings between VH1 and VH2. This leads to a  $6 \times 6$  matrix  $H_{\text{eff}}(\mathbf{k}, \Delta)$  corresponding to the six patches at VH1 and VH2 near the three  $M$  points. By performing a Taylor expansion in  $\mathbf{k}$  and keeping leading order terms, we obtain  $H_{\text{eff}}$  in Eq. (2) with parameters  $\epsilon_1 = 6.16$  eV,  $\epsilon_2 = 6.40$  eV,  $b = 0.52$ ,  $b' = 0.96$ ,  $\lambda = 0.35$  eV  $\text{\AA}$ , where  $a = 5.48$   $\text{\AA}$  is the lattice constant. Because the wave functions at both vHSs have significant weight on  $\tilde{d}$  orbitals, the coupling  $\lambda$  between the two vHSs receives major contribution from the hopping amplitude  $t_{dd}$  between nearest-neighbor  $\tilde{d}$  orbitals; hence,  $\lambda$  is generally nonzero. With a finite  $\lambda$ , the above theory for LCBO is applicable to  $\text{AV}_3\text{Sb}_5$ , indicating that the LCBO phase can be stabilized as the ground state.

*Phase diagram of CDW orders.*—The phase diagram of  $H_{\text{eff}}$  obtained by minimizing the free energy with respect to  $\Delta$  at different chemical potential and interaction strength is shown in Fig. 4(a). The LCBO phase is more pronounced near VH2 due to the difference in wave function structures at VH1 and VH2. Equation (4) requires the eigenvalues  $E_{1-3}$  be negative and  $E_{4-6}$  be positive. Based on Eq. (3), these conditions lead to  $4|b'|^2|\Delta| > \delta\epsilon$  when  $\mu \sim \epsilon_2$ , while when  $\mu \sim \epsilon_1$  they lead to  $4|b|^2|\Delta| > \delta\epsilon$ . Since  $|b'| > |b|$

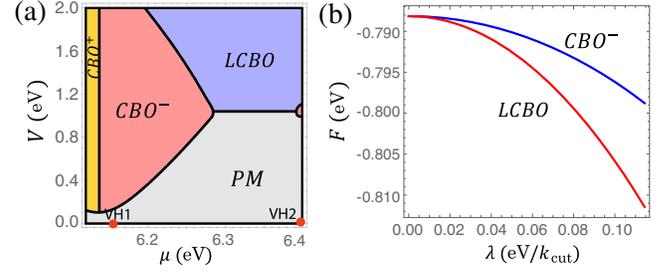


FIG. 4. (a) Phase diagram of  $H_{\text{eff}}$  at different interaction strengths and chemical potential with parameters  $\epsilon_1 = 6.16$  eV,  $\epsilon_2 = 6.40$  eV,  $b = 0.52$ ,  $b' = 0.96$ ,  $\lambda k_{\text{cut}} = 0.1$  eV and temperature is 90 K.  $PM$  refers to the pristine metal without any CDW order. (b) Free energy of LCBO and  $CBO^-$  as a function of coupling  $\lambda$  at a fixed interaction strength. It shows LCBO is favored at finite  $\lambda$ .

due to the larger weight of  $\tilde{d}$  orbital at VH1, when  $\mu \sim \epsilon_2$  it requires smaller  $|\Delta|$  and smaller interaction to realize LCBO. This leads to the smaller critical interaction strength near VH2 as shown in the phase diagram. The competition between  $CBO^-$  and LCBO depends on the strength of  $\lambda$ . The free energy of the  $CBO^-$  and LCBO phases at  $\mu = \epsilon_2$ ,  $V = 1.3$  eV as a function of coupling strength  $\lambda$  is shown in Fig. 4(b). It shows LCBO and  $CBO^-$  are degenerate when  $\lambda = 0$ , and a finite  $\lambda$  makes the free energy of LCBO lower than  $CBO^-$ , consistent with Eq. (4).

*Effects of the other bands.*—In  $\text{AV}_3\text{Sb}_5$  there are other bands near the Fermi level and their effects need to be investigated. For this purpose, we consider an effective patch model obtained by adding one more band below VH1 (denoted as  $\epsilon_3$ ) in Fig. 3(a) to  $H_{\text{eff}}$ , which expands it to a  $9 \times 9$  matrix near the  $M$  points. This model includes VH1, VH2, and  $\epsilon_3$ , and its phase diagram is shown in Fig. 5(a). Compared with Fig. 4(a), which only includes VH1 and VH2, the key variation in Fig. 5(a) occurs near VH1, which is close to the additional band at  $\epsilon_3$ . However, in regions around VH2 that are more distant from  $\epsilon_3$ , the two phase diagrams resemble each other, with LCBO emerging in

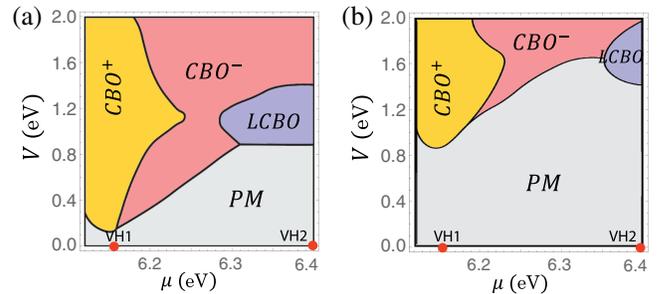


FIG. 5. (a) Phase diagram of the effective patch model obtained by including VH1, VH2, and  $\epsilon_3$ .  $PM$  refers to the pristine metal without any CDW order. (b) Phase diagram that takes into account all bands in  $H_{\text{TB}}$  and the momentum summation is over the Brillouin zone. The LCBO phase still exists near VH2.

both scenarios. We further demonstrate that the emergence of LCBO inferred from the patch model remains valid when all the bands in the tight binding model are considered and the momentum cutoff is removed. The phase diagram obtained with all bands in  $H_{\text{TB}}(\mathbf{k})$  included is shown in Fig. 5(b). The real space configuration of these phases are shown in Fig. 2 with the order parameter given in Eq. (1). The summation of momentum in computing the free energy is taken over the whole Brillouin zone. The LCBO phase exists near VH2, whereas near VH1 the ground state is CBO, due to the effect of band structure away from  $M$  points and the other bands that are not taken into account in the patch models. This comparison suggests despite the quantitative difference in these phase diagrams, our main finding of LCBO remains valid in the full-band model as long as the chemical potential is near VH2.

*Discussion.*—We provide a mechanism to realize LCBO in kagome systems based on the coupling between multiple vHSs with different mirror symmetries. The imaginary part of LCBO breaks time-reversal symmetry, whereas the real part of LCBO can induce lattice distortion with star of David or trihexagonal patterns. Experiments on  $\text{AV}_3\text{Sb}_5$  have observed staggered patterns of lattice distortion among different kagome layers [26]. If the ground state is described by LCBO, we expect the loop current order to be staggered along the  $c$  axis as well. Our theory shows LCBO is more favorable when the energy difference  $\delta\epsilon$  between vHSs is small. Experiments and first-principle computations suggest that pressure can lead to an increase of  $\delta\epsilon$  [45,72]; hence, we expect LCBO to disappear under high pressure, which is consistent with the disappearance of CDW under high pressure observed in experiments [31,48,65,70]. The phase diagram of  $\text{AV}_3\text{Sb}_5$  in Fig. 5(b) suggests that LCBO emerges when the chemical potential is close to VH2. Thus we predict that electron doping the material is more likely to induce the LCBO phase. Given the general applicability of our theory to kagome systems having vHSs with distinct mirror eigenvalues, we hope this work will inspire further exploration of kagome materials with mirror symmetries.

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