Article

Optical Conductivity on Charge Order Transition in Organic Dirac Electron System α-(BEDT-TTF)$_2$I$_3$

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Abstract: The optical conductivity in the charge order phase is calculated in the extended Hubbard model describing an organic Dirac electron system α-(BEDT-TTF)$_2$I$_3$ using the mean field theory and the Nakano-Kubo formula. A peak structure due to interband excitation being characteristic in two-dimensional Dirac electron system is found above the charge order gap. It is shown that the peak structure originates from the Van Hove singularities of the conduction and valence bands, where those singularities are located at a saddle point between two Dirac cones in momentum space. The frequency of the peak structure exhibits drastic change in the vicinity of the charge order transition.

Keywords: Dirac electron; charge order; optical conductivity; organic conductor; α-(BEDT-TTF)$_2$I$_3$

1. Introduction

An organic conductor α-(BEDT-TTF)$_2$I$_3$ has attracted many interests, since it exhibits a transition between the charge order (CO)[1–6] and the massless Dirac electron (massless DE) [7–14] as hydrostatic pressure, P, increases. Recently, strong electron correlation effects have been revealed in both the CO[15] and the massless DE[16–19] in spin fluctuations. Thus electron correlation effects in transport phenomena have been also expected, especially in crossover region between the CO and the massless DE.

It has been observed that the optical gap determined by the optical conductivity decreases monotonously as P increases and reaches almost zero at about $P_c = 12$kbar[20,21], while the resistivity gap reaches almost zero at about 7kbar[22]. In order to explain such metallic behavior in the presence of the CO gap, metallic channels owing to edges and domain walls in the CO have been studied using the extended Hubbard model[23–26]. It has been shown that the massive DE phase with the gapless edge states emerges in the intermediate region between the massless DE phases and the trivial CO. Although the CO gap induced by the inversion symmetry breaking exists in both the massive DE phase and the trivial CO, a pair of Dirac cones with a finite gap at incommensurate momentum, $\pm k_{\mathrm{D}}$, merges at a time reversal invariant momentum (TRIM) at the transition between these two phases[11,14,27,28]. Such a drastic change in the band structure is expected to give rise to a characteristic in the optical conductivity.

In the present paper, the optical conductivity is calculated in the band structure determined by the mean-field theory in the extended Hubbard model for the two dimensional electron system in the organic conductor α-(BEDT-TTF)$_2$I$_3$, where the CO transition is controlled by the nearest-neighbor Coulomb repulsion, V_a. It is shown that a peak structure emerges above the CO gap in the optical conductivity. The frequency of the peak structure, ω_{peak}, owing to interband excitation between two Van Hove singularities in the conduction and valence bands, rapidly moves as a nonmonotonic function of V_a, while the frequency of the CO gap, ω_{CO}, increases monotonically as V_a increases. Those Van Hove singularities originate from the saddle points between two Dirac cones. The optical conductivity exhibits a characteristic strong peak when two Dirac cones merge in the presence of a large CO gap.

This paper is described as follows. An extended Hubbard model for two dimensional electron system in α-(BEDT-TTF)$_2$I$_3$, the mean field theory, and the optical conductivity are described in section 2. Numerical results are shown in section 3. Section 4 and 5 are devoted to discussion and summary.

2. Formulation

The extended Hubbard model[1,2] has been used in theoretical studies for α-(BEDT-TTF)$_2$I$_3$, in order to take the on-site Coulomb repulsion, U, and the nearest-neighbor Coulomb repulsions, $V_{\alpha\beta}$, into account.

$$\begin{aligned} H &= \sum_{(i\alpha,j\beta),\sigma} (t_{(i\alpha,j\beta)}\, a^\dagger_{i\alpha\sigma} a_{j\beta\sigma} + \text{h.c.}) \\ &+ \sum_{i\alpha} U\, a^\dagger_{i\alpha\uparrow} a^\dagger_{i\alpha\downarrow} a_{i\alpha\downarrow} a_{i\alpha\uparrow} \\ &+ \sum_{(i\alpha:j\beta)} \sum_{\sigma,\sigma'} V_{i\alpha j\beta}\, a^\dagger_{i\alpha\sigma} a^\dagger_{j\beta\sigma'} a_{j\beta\sigma'} a_{i\alpha\sigma}, \end{aligned} \tag{1}$$

where $a_{i\alpha\sigma}$ and $t_{(i\alpha,j\beta)}$ represent the annihilation operators and the transfer energies with unit cells i, j, spins σ, and sublattices $\alpha, \beta =$ A, A′, B and C of α-(BEDT-TTF)$_2$I$_3$.

Hereafter, the energies are given in eV. The tight binding model for α-(BEDT-TTF)$_2$I$_3$[29–33] is shown in Fig. 1(a). The sublattice A and A′ are equivalent due to the inversion symmetry in the massless DE phase. The transfer energies given by the first-principle calculation[32]: $t_{b1} = 0.1241, t_{b2} = 0.1296, t_{b3} = 0.0513, t_{b4} = 0.0152, t_{a1} = -0.0267, t_{a2} = -0.0511, t_{a3} = 0.0323, t'_{a1} = 0.0119, t'_{a3} = 0.0046$, and $t'_{a4} = 0.0060$. The nearest neighbor interaction V_a in the stacking direction is used for controlling the CO transition, because this is the most sensitive as a function of P[34–36], while we treat $U = 0.4$ and $V_b = 0.05$ as constants. The temperature $T = 0.001$ is fixed in the present paper. The lattice constants, k_B and $\hbar$ are taken as unity. The system size in numerical calculations is $N_L = 500$.

The mean-field Hamiltonian H_MF[10] is

$$H_\mathrm{MF} = \sum_{\mathbf{k}\alpha\beta\sigma} \tilde{\epsilon}_{\alpha\beta\sigma}(\mathbf{k}) a^\dagger_{\mathbf{k}\alpha\sigma} a_{\mathbf{k}\beta\sigma}, \tag{2}$$

$$\tilde{\epsilon}_{\alpha\beta\sigma}(\mathbf{k}) = \phi_{\alpha\sigma}\delta_{\alpha\beta} + \epsilon_{\alpha\beta}(\mathbf{k}), \tag{3}$$

$$\phi_{\alpha\sigma} = U_\alpha \langle n_{\alpha-\sigma}\rangle + \sum_{\beta'\sigma'} V_{\alpha\beta'} \langle n_{\beta'\sigma'}\rangle, \tag{4}$$

$$\epsilon_{\alpha\beta}(\mathbf{k}) = \sum_\delta t_{\alpha\beta} e^{i\mathbf{k}\cdot\delta}, \tag{5}$$

where $\phi_{\alpha\sigma}$ is the Hartree potential, $\langle n_{\alpha\sigma}\rangle = \langle a^\dagger_{i\alpha\sigma} a_{i\alpha\sigma}\rangle$ is the electron number, and δ is a vector between unit cells. The energy eigenvalues $\xi_{\gamma\sigma}(\mathbf{k})$ and the wave functions $\Phi_{\alpha\gamma\sigma}(\mathbf{k})$ are given by

$$\sum_\beta \tilde{\epsilon}_{\alpha\beta\sigma}(\mathbf{k})\, \Phi_{\beta\gamma\sigma}(\mathbf{k}) = \xi_{\gamma\sigma}(\mathbf{k})\, \Phi_{\alpha\gamma\sigma}(\mathbf{k}), \tag{6}$$

with the band index $\gamma = 1, 2, 3, 4$. The conduction and valence bands correnspond to $\xi_{1\sigma}(\mathbf{k})$ and $\xi_{2\sigma}(\mathbf{k})$, respectively, since the Fermi energy is located between these two bands. The electron number $\langle n_{\alpha\sigma}\rangle$ is given by

$$\langle n_{\alpha\sigma}\rangle = \sum_{\mathbf{k}\gamma} |\Phi_{\alpha\gamma\sigma}(\mathbf{k})|^2 f(\xi_{\gamma\sigma}(\mathbf{k})), \tag{7}$$

where the Fermi distribution function is $f(\xi_{\gamma\sigma}(\mathbf{k})) = 1/(\exp[(\xi_{\gamma\sigma}(\mathbf{k}) - \mu)/k_B T] + 1)$ with the chemical potential μ determined so that the bands are 3/4-filled.

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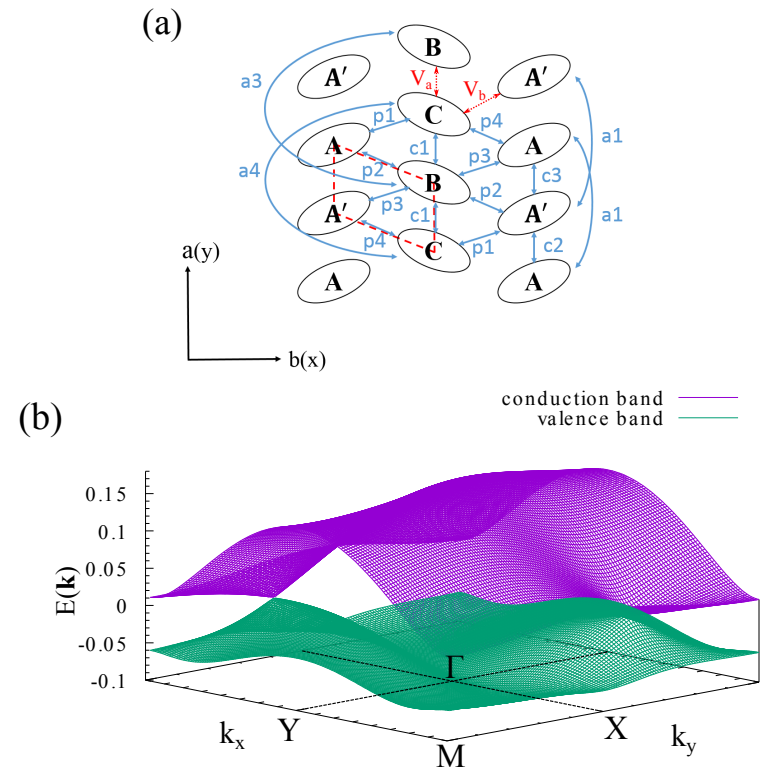

Figure 1. Schematic figure of a unit cell with transfer energies, on-site Coulomb repulsion U and the nearest-neighbor Coulomb repulsions, V_a and V_b (a). The conduction band (purple) and valence band (green) in the massive DE phase for $V_a = 0.18$ (b).

The Green function $G_{\alpha\beta\sigma}(\omega, \mathbf{k})$ and the density of state $\rho(\omega)$ are given by

$$G_{\alpha\beta\sigma}(\omega, \mathbf{k}) = \sum_{\gamma} \frac{\Phi^*_{\alpha\gamma\sigma}\Phi_{\beta\gamma\sigma}}{\hbar\omega - (\xi_{\gamma\sigma}(\mathbf{k}) - \mu) + i\delta}, \tag{8}$$

$$\begin{aligned}\rho(\omega) &= \frac{1}{N_L}\sum_{\mathbf{k}\alpha\sigma}\left(-\frac{1}{\pi}\mathrm{Im}G_{\alpha\alpha\sigma}(\omega, \mathbf{k})\right) \\ &= \frac{1}{N_L}\sum_{\mathbf{k}\alpha\gamma\sigma}\delta(\hbar\omega - \xi_{\gamma\sigma}(\mathbf{k}))|\Phi_{\gamma\alpha\sigma}(\mathbf{k})|^2,\end{aligned} \tag{9}$$

where N_L is the number of lattice points.

The optical conductivity is calculated by the Nakano-Kubo formula based on linear response theory. It is represented by

$$\sigma(\omega) = \frac{1}{i\omega}\left[K(\omega) - K(0)\right], \tag{10}$$

$$K(\omega) = -\frac{1}{N_L}\left(\frac{e}{\hbar}\right)^2 \sum_{\mathbf{k}\gamma\gamma'\sigma} |\mathrm{v}_{\gamma\gamma'\sigma}(\mathbf{k})|^2 \frac{f(\xi_{\gamma\sigma}(\mathbf{k})) - f(\xi_{\gamma'\sigma}(\mathbf{k}))}{\xi_{\gamma\sigma}(\mathbf{k}) - \xi_{\gamma'\sigma}(\mathbf{k}) + \omega + i\delta}, \tag{11}$$

where the velocity matrix $\mathrm{v}_{\gamma\gamma'\sigma}$ is calculated by

$$\mathrm{v}_{\gamma\gamma'\sigma}(\mathbf{k}) = \sum_{\alpha\beta}\Phi^*_{\alpha\gamma\sigma}(\mathbf{k})v_{\alpha\beta\sigma}(\mathbf{k})\Phi_{\beta\gamma'\sigma}(\mathbf{k}), \tag{12}$$

$$v_{\alpha\beta\sigma}(\mathbf{k}) = \frac{1}{\hbar}\frac{\partial}{\partial\mathbf{k}}\epsilon_{\alpha\beta\sigma}(\mathbf{k}). \tag{13}$$

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3. Results

Figure 1(b) shows the conduction and valence bands in the massive DE phase. There is a pair of massless Dirac cones at incommensurate momenta, $\pm k_{\rm D}$. The Fermi energy is located at the degenerate points of the two bands. There are several saddle points at the TRIMs near the Fermi energy, *e. g.*, the M-point in the conduction band (Mc-VHS), the M-point in the valence band (Mv-VHS), and the Y-point in the valence band (Yv-VHS).

The optical conductivities at several V_a are shown in Fig. 2(a). These values are divided by the universal conductivity $\sigma_0 = \pi e^2/2h$ [37]. In the massless DE phase for $V_a = 0.18$, the optical conductivity almost reaches a universal constant for $T < \omega < \Lambda$, where $\Lambda \cong 0.01$ is a energy scale of the linear dispersion as shown in previous studies for the massless DE[37–40]. When $V > V_a^{c1} = 0.198$, a frequency of the CO gap, $\omega_{\rm CO}$, increases as V_a increases as shown in Fig. 2(b), where $\omega_{\rm CO}$ is defined as a flexion point of the shoulder structure in the optical conductivity. It is found that a peak structure appears above $\omega_{\rm CO}$ and its frequency, $\omega_{\rm peak}$, rapidly decreases as V_a increases for $V_a < V_a^{c2} = 0.212$, which is defined by the merging of the Dirac cones in the conduction band[25,26]. $\omega_{\rm peak}$ rebounds after falling to $\omega_{\rm CO}$, and the optical conductivity shows a strong peak. Those two frequencies exhibits asymptotic behavior for $V_a > V_a^{c2}$.

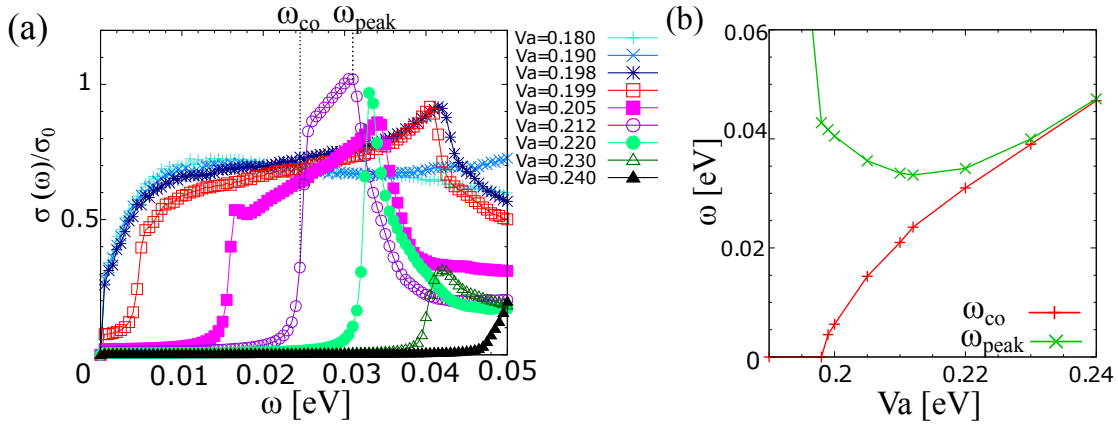

Figure 2. The optical conductivities divided by the universal conductivity $\sigma_0 = \pi e^2/2h$[37] for $V_a = 0.180, 0.190, 0.198, 0.199, 0.205, 0.212, 0.220, 0.230, 0.240$ (a). $\omega_{\rm CO}$ and $\omega_{\rm peak}$ for $V_a = V_a^{c2} = 0.212$ are shown in (a). V_a-dependences of $\omega_{\rm CO}$ and $\omega_{\rm peak}$ are shown in (b). A characteristic peak structure is found near the CO transition in the extended Hubbard model describing the organic Dirac electron system α-(BEDT-TTF)$_2$I$_3$.

Figure 3 shows the density of states $\rho(\omega)$, where the Fermi energy is defined as zero. When $V_a < V_a^{c1}$, there is a valley due to the Dirac cones. A CO gap, $\omega_{\rm CO}$, opens at the Fermi energy for $V > V_a^{c1}$. There are several Van Hove singularities (VHS) due to saddle points of the conduction and valence bands (see Fig. 1(b)). Here we pay attention to VHS at the M-point in the conduction band (Mc-VHS) and that in the valence band (Mv-VHS), respectively. The Mc-VHS stays an energy for $V_a < V_a^{c2}$. Its energy rapidly increases and the peak structure disappears for $V_a > V_a^{c2}$, since it is absorbed by the upper edge of the CO gap, owing to the merging of the Dirac cones in the conduction band as shown in Fig. 4. The Mv-VHS, on the other hand, moves very rapidly until it reaches the lower edge of the CO gap at V_a^{c2}. The Mv-VHS and the lower edge of the CO gap exhibits asymptotic behavior for $V_a > V_a^{c2}$. An energy difference between the Mc-VHS and Mv-VHS coincides with $\omega_{\rm peak}$ in the optical conductivity shown in Fig. 2(a). Other VHSs, *e. g.*, VHS at the Y-point in the valence band (Yv-VHS), show completely different behavior as V_a increases.

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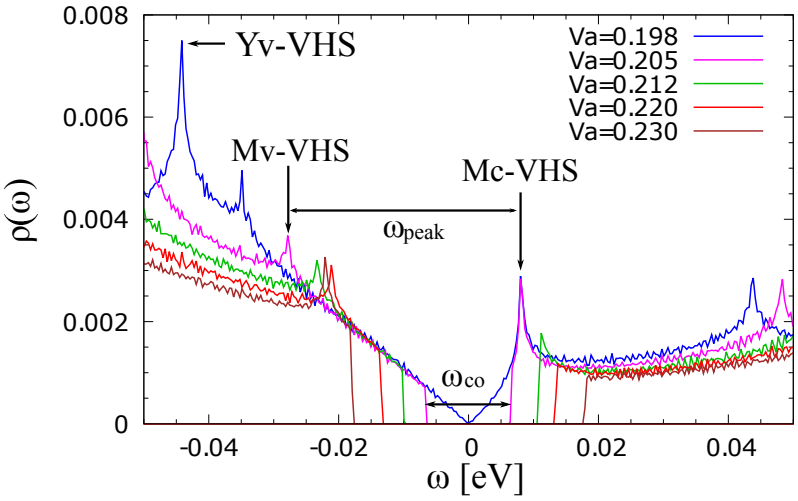

Figure 3. The density of states $\rho(\omega)$ for $V_a = 0.198, 0.205, 0.212, 0.220, 0.230$. The origin of the peak structure in the optical conductivity is identified.

In order to analyze the behavior of ω_{peak} and ω_{CO}, the band structure is intensively examined in Fig. 4. Both Mc-VHS and Mv-VHS exist at the M-point (the saddle point) between two Dirac cones. The Dirac cones in the conduction band (the purple band) merge at the M-point at V_a^{c2} in the presence of large CO gap as shown in Figs. 4(b) and 4(e), leading to the absorption of the Mc-VHS into the upper edge of the CO gap. On the other hand, the massive Dirac cones in the valence band (the green band) do not merge against relatively larger V_a as shown in Figs. 4(c) and 4(f), since the Dirac cones are tilted[11,12]. Thus the Mv-VHS and the lower edge of the CO gap shows asymptotic behavior.

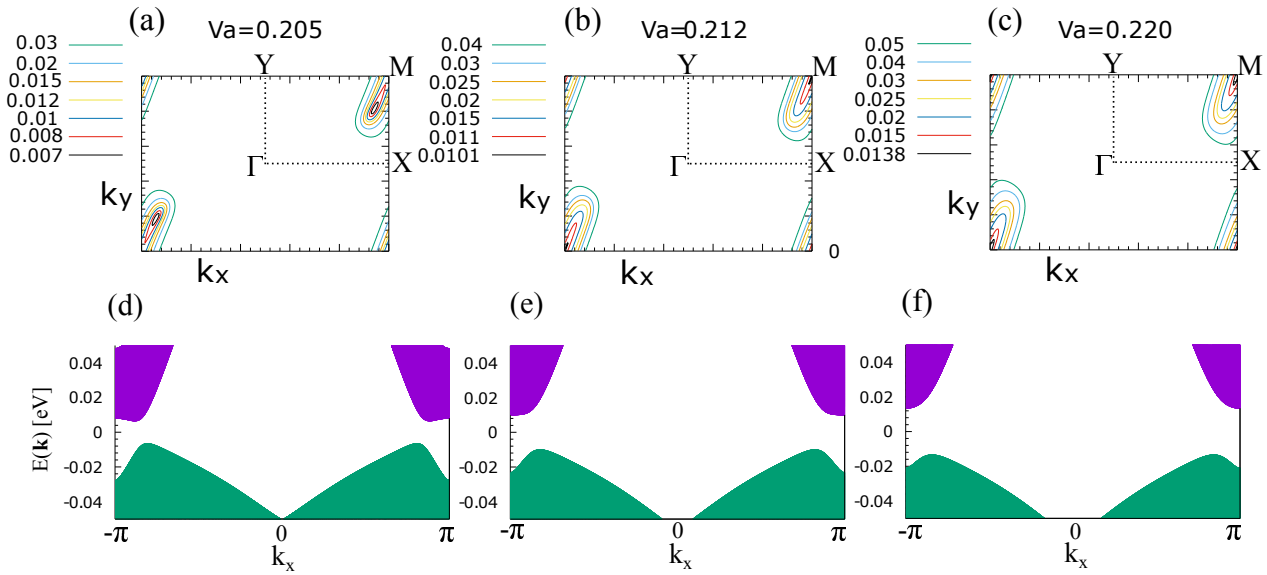

Figure 4. The contour plots of the conduction band for $V_a = 0.205$ (a), $V_a = V_a^{c2} = 0.212$ (b), and $V_a = 0.220$ (c). The band structures as a function of k_x for $V_a = 0.205$ (d), $V_a = V_a^{c2} = 0.212$ (e), and $V_a = 0.220$ (f), where the CO gaps open between the conduction bands (the purple bands) and the valence bands (the green bands). Tilting of the Dirac cones causes electron-hole asymmetric behavior as the CO gap increases.

4. Discussion

The drastic change of the optical conductivity near CO transition is characterized not only the CO gap, but also the peak structure as shown in Fig. 2(a) and 2(b). By careful analysis on the $\rho(\omega)$ shown

in Fig. 3 and band structure shown in Fig. 4, it is elucidated that the origin of the peak structure is the VHSs at the M-points between two tilted Dirac cones. The nonmonotonic V_a-dependence of $\omega_{\rm peak}$ is due to both the merging of the Dirac cones with the CO gap and the tilting of the Dirac cones. Those characteristic may be measured in the low frequency region of the optical conductivity[20], which can provide many important information on existence, merging, and tilting of the two-dimensional massive Dirac electrons in the CO phase.

5. Conclusions

The optical conductivity in the vicinity of the CO transition has been investigated using the Nakano-Kubo formula and the mean-field theory in the extended Hubbard model describing the Dirac electrons in α-(BEDT-TTF)$_2$I$_3$. It has been found that a peak structure above the CO gap emerges due to the two dimensional Dirac cones. It has been also shown that the drastic change of the peak structure in the vicinity of the CO transition indicates the merging of the massive Dirac electrons.

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Conflicts of Interest: The authors declare no conflict of interest.

Abbreviations

The following abbreviations are used in this manuscript:

DE	Dirac electron
CO	charge order
VHS	Van Hove singularity
DOS	density of states
TRIM	time reversal invariant momentum
Mc-VHS	Van Hove singularity at the M-point in the conduction band
Mv-VHS	Van Hove singularity at the M-point in the valence band
Yv-VHS	Van Hove singularity at the Y-point in the valence band

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