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Effects of electron correlation on the band gap of a chain of halogen-bridged transition-metal compounds

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The effect of electron correlation on the band gap of the halogen-bridged transition-metal compounds (*MX* complexes) with charge-density waves is studied by using the projection technique. It is found that the band gap of an *MX* complex is reduced by the electron correlation. This effect in an *MX* complex is contrary to that in polyacetylene, where the band gap of the bond-order wave is enhanced by the electron correlation, and the origin for this contrast is discussed.

In recent years, many studies have focused on the halogen-bridged mixed-valence transition-metal compounds (*MX* complexes),[1–3] both because of the interesting properties produced by the competition and cooperation of the electron-phonon (*e-p*) and electron-electron (*e-e*) interactions, and because of their potential applications in nonlinear optics.[4] In 1991, Iwasa *et al.*[5] successfully measured the third-harmonic generation (THG) $\chi^{(3)}$ of PtCl, in which the ground state has strong *M* charge disproportionation and large structural distortion of the *X* sublattice, i.e., the charge-density-wave ground state. Although the observed $\chi^{(3)}$ of PtCl is not large enough for practical use, the THG of the *MX* complex is able to be enhanced by properly controlling the competition between the *e-p* and *e-e* interactions,[4] which can be changed almost continuously by chemically varying the transition metal *M*, halogen *X*, and ligand *L*. Since the THG is sensitively dependent on the optical gap E_g ($\chi^{(3)} \sim E_g^{-6}$), and the gap is governed by both the *e-p* and *e-e* interactions. Thus it is necessary to study the effect of the *e-e* interaction on the band gap, which is produced by the *e-p* interaction. This effect can be used to enhance the THG of the *MX* complex.

The band gap, which is the excitation energy to remove an electron from the top of the valence band to the bottom of the conduction band, is strongly dependent on the electron correlation. From the physical picture, if the correlation is considered, the energy of the mean-field ground state is lowered due to the spontaneous creation and annihilation of the electron-hole pairs. When an extra electron or hole is introduced, there is a cloud of hole (electron) around this electron (hole), and it results in the *gain* of polarization energy which reduces the excitation energy. Meanwhile, the extra electron or hole makes the number of possible intermediate states by the spontaneous excitation less due to the Pauli principle; it gives rise to the *loss* of the correlation energy of the ground state. Recently, Wu[6] applied the projection technique, which had been developed by Becker and Fulde[7] to study the band gap of the polymer, and found that for the Hubbard interaction, the electron correlation enhanced the band gap. Naturally, people want to know how the electron correlation affects the band gap in the *MX* complex. The answer is not obvious because the ground states of the *MX* complex and polymer are different due to the different *e-p* coupling, the charge-density wave (CDW) in the former and the bond-order wave (BOW) in the latter, although there are many similarities between these two materials. In fact, our calculations of second-order perturbation have shown that the electron correlation reduces the mean-field band gap of the *MX* complex,[8] but the result is valid only in weak *e-e* interaction; therefore it is needed to go beyond the perturbation. In this paper, we shall examine the correlation effect on the band gap of the *MX* complex by applying the projection technique, which is applicable when the interaction is not weak.

For simplicity, the *MX* complex is considered as a chain of alternating *M* and *X* atoms. In the one-band model, *M* has an unpaired electron in the d_{z^2} orbital (z is parallel to the chain) and this orbital makes an energy band through the supertransfer between neighboring orbitals. However, the displacement of *X* modulates the energy levels of d_{z^2}, and it causes a coupling between the electrons and the phonons. The Hamiltonian of this system is[3]

$$\hat{H} = -T\sum_{i\sigma}(c_{i\sigma}^\dagger c_{i+1\sigma} + \text{H.c.}) + \omega\sum_i q_i^2/2 + \sqrt{S}\omega\sum_{i\sigma}(q_i - q_{i+1})n_{i\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}\ , \tag{1}$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) denotes the creation (annihilation) operator of an electron with spin σ at site i, and $n_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}$. T is the transfer energy of an electron between two neighboring metallic sites. ω is the phonon energy of the halogen ion, q_i is its dimensionless coordinate and describes the motion of *X* parallel to the chain; its kinetic energy is neglected according to the adiabatic approximation. S is the *e-p* coupling energy, while U denotes the on-site Hubbard repulsions. Introducing Q_i ($\equiv\sqrt{\omega/S}q_i$), $\hat{h}$ ($\equiv\hat{H}/T$), s ($\equiv S/T$), and u ($\equiv U/T$), we can rewrite Eq.

(1) in a dimensionless form as

$$\hat{h} = -\sum_{i\sigma}(c_{i\sigma}^\dagger c_{i+1\sigma} + \text{H.c.}) + s\sum_i Q_i^2/2 + s\sum_{i\sigma}(Q_i - Q_{i+1})n_{i\sigma} + u\sum_i n_{i\uparrow}n_{i\downarrow} . \quad (2)$$

The ground state has uniformly dimerized configuration, and we denote $Q_i = (-1)^i\bar{v}$, $\bar{v}$ is the dimerization amplitude. In momentum space, the Hamiltonian has the following form:

$$\hat{h} = \sum_{k\sigma}\epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + 2s\bar{v}\sum_{k\sigma} c_{k\sigma}^\dagger c_{k-Q\sigma} + I\sum_{k,k',q} c_{k\uparrow}^\dagger c_{k+q\uparrow} c_{k'\downarrow}^\dagger c_{k'-q\downarrow} + \tfrac{1}{2}Ns\bar{v}^2 , \quad (3)$$

where $c_{k\sigma} = (1/\sqrt{N})\sum_l e^{-ikl}c_{l\sigma}$, $\epsilon_k = -2\cos k$, $Q = \pi$, and $I = u/N$.

When *e-p* coupling is dominant compared to *e-e* repulsion, the ground state is the CDW state. To consider electronic correlation, we should first study the *e-e* interaction in the mean-field theory (MFT). The CDW-type mean-field Hamiltonian can be written as[8]

$$\hat{h}_{\text{MF}} = \sum_{k\sigma}{}' \Psi_{k\sigma}^\dagger \mathcal{H}\Psi_{k\sigma} + \tfrac{1}{2}Ns\bar{v}^2 - NW^2/u , \quad (4)$$

where the prime means that the sum ranges over the positive half of the Brillouin zone. The order parameter W has been defined as

$$W = I\sum_{k\sigma}{}' \langle c_{k\sigma}^\dagger c_{k+Q\sigma}\rangle , \quad (5)$$

and we have also introduced the spinor $\Psi_{k\sigma} = (c_{k\sigma}, c_{k-Q\sigma})^T$. The one-particle Hamiltonian $\mathcal{H}$ is a 2×2 matrix,

$$\mathcal{H} = \begin{bmatrix} \epsilon_k & \Delta \\ \Delta & -\epsilon_k \end{bmatrix} ,$$

where $\Delta = 2s\bar{v} + W$. The mean-field electronic Hamiltonian can be diagonalized easily, yielding

$$\hat{h}_0^e = \sum_{k\sigma}{}' E_k(A_{k\sigma}^\dagger A_{k\sigma} - B_{k\sigma}^\dagger B_{k\sigma}) , \quad (6)$$

with

$$E_k = \sqrt{\epsilon_k^2 + \Delta^2} . \quad (7)$$

$A_{k\sigma}$ and $B_{k\sigma}$ annihilate an electron in the conduction and the valence band, respectively. They can be expressed by $c_{k\sigma}$ and $c_{k-Q\sigma}$,

$$\begin{bmatrix} A_{k\sigma} \\ B_{k\sigma} \end{bmatrix} = \begin{bmatrix} u_k & -v_k \\ v_k & u_k \end{bmatrix} \begin{bmatrix} c_{k\sigma} \\ c_{k-Q\sigma} \end{bmatrix} , \quad (8)$$

where $u_k = [(E_k + \epsilon_k)/2E_k]^{1/2}$ and $v_k = -[(E_k - \epsilon_k)/2E_k]^{1/2}$. This MFT indicates the band gap is 2Δ, which satisfies the relation[8]

$$1/8s - u = (1/\pi\sqrt{4+\Delta^2})K(2/\sqrt{4+\Delta^2}) , \quad (9)$$

$K(x)$ is the first-kind complete elliptic integrals.

To consider the effect of electron correlation, we should split the total electronic Hamiltonian into two terms,

$$\hat{h}^e = \hat{h}_0^e + \hat{h}_1 , \quad (10)$$

$\hat{h}_0^e$ is our mean-field electronic Hamiltonian and $\hat{h}_1$ is a two-particle interaction term. If we divide the operator c_{ls} into two parts, i.e., the electron operator in conduction band a_{ls} and the hole operator in valence band $b_{ls}^\dagger$, the two-particle part of the Hubbard interaction can be written as[9]

$$\hat{h}_1 \equiv \frac{u}{2}O = \frac{u}{2}[O^{(1)} + (O^{(2)} + \text{H.c.}) + (O^{(3)} + \text{H.c.})] , \quad (11)$$

where

$$O^{(1)} = \sum_{lss'}[a_{ls}^\dagger a_{ls'}^\dagger a_{ls'}a_{ls} + b_{ls}^\dagger b_{ls'}^\dagger b_{ls'}b_{ls} - 2a_{ls}^\dagger b_{ls'}^\dagger b_{ls'}a_{ls} + 2a_{ls}^\dagger b_{l\bar{s}}^\dagger b_{l\bar{s}'}a_{ls'}] \quad (12a)$$

is the interaction between electron-electron, hole-hole, and electron-hole,

$$O^{(2)} = \sum_{lss'} a_{ls}^\dagger a_{ls'}^\dagger b_{l\bar{s}'}^\dagger b_{l\bar{s}}^\dagger \quad (12b)$$

is the spontaneous creation of two electron-hole pairs, and

$$O^{(3)} = 2\sum_{lss'}[a_{ls}^\dagger a_{ls'}^\dagger b_{l\bar{s}'}^\dagger a_{ls} + b_{ls}^\dagger b_{ls'}^\dagger a_{l\bar{s}'}^\dagger b_{ls}] \quad (12c)$$

is the creation of an electron-hole pair through the scattering of an electron or a hole.

In the CDW ground state, the lattice configuration is uniformly dimerized and there is the symmetry between electron and hole.[10] We only consider the case of an electron added to the half-filled system. The excitation energy is defined by

$$\varepsilon(k) = E_1(k) - E_0 , \quad (13)$$

E_0 is the energy for the ground state of the half-filled system and $E_1(k)$ is the energy for the system with an extra electron which has wave number k.

To use the projection technique, at first, one must divide the Liouville space R into a relevant part R_0 spanned by a set $\{A_\nu\}$ and a remaining part R_1. The approximation is that the operators are projected into the R_0 and the calculation is carried out within the R_0. The key issue is how to select the relevant space R_0 to determine the excitation energies $\varepsilon(k)$ as accurately as possible. As we have mentioned before, the main contribution to the band gap, considering electronic correlation, comes from two aspects: one is the blocking of the spontaneous excitations of electron-hole pairs if these excitations are associated with the extra particle (we use S_μ^η), the other is the excitation of electron-hole pairs through the scattering of the extra particle (we use S_μ^π), the former gives rise to a *loss* of the correlation energy in the ground state so that the excitation energy is increased and the latter is a polarization process, which decreases the excitation energy by the *gain* of the polarization energy. So we get $\{A_\mu\} = \{a_{ks}^\dagger\} \oplus \{S_\mu^\pi a_{ks}^\dagger\} \oplus \{a_{ks}^\dagger S_\mu^\eta\}$, where $a_{ks}^\dagger$ creates an electron ($A_{ks}^\dagger$) or a hole ($B_{k\bar{s}}$); then we can write the excitation energies as two parts

$$\varepsilon(k)=E_k+\varepsilon^{\text{corr}}(k)\ , \tag{14}$$

here E_k is the excitation energy of MFT, $\varepsilon^{\text{corr}}(k)$ is the correction to the MFT results after considering correlation and it can be split into two parts as physical picture,[6]

$$\varepsilon^{\text{corr}}(k)=\varepsilon^{\pi}(k)+\varepsilon^{\eta}(k)\ , \tag{15}$$

$\varepsilon^{\pi}(k)$ is the *gain* of polarization energy and $\varepsilon^{\eta}(k)$ is the *loss* of the correlation energy in the ground state. The explicit expressions of $\varepsilon^{\pi}(k)$ and $\varepsilon^{\eta}(k)$ can be found in Ref. 6. We also neglected $(S^{\pi}_{\mu}a^{\dagger}_{ks}|\hat{h}_1 a^{\dagger}_{ks}S^{\eta}_{\nu})$, since it is believed that the interaction between these two kinds of correlation effects is small as long as the *e-e* repulsion is not very strong. The polarization scattering operator S^{π}_{μ} and the correlation excitation operator S^{η}_{μ} are written as follows:

$$S^{\pi}_{ij}=\tfrac{1}{2}\sum_{\sigma\sigma'} a^{\dagger}_{i\sigma}b^{\dagger}_{i\bar{\sigma}}a^{\dagger}_{j\sigma'}a_{j\sigma'}\ , \tag{16a}$$

$$S^{\eta}_{ij}=\tfrac{1}{2}\sum_{\sigma\sigma'} a^{\dagger}_{i\sigma}b^{\dagger}_{i\bar{\sigma}}a^{\dagger}_{j\sigma'}b^{\dagger}_{j\bar{\sigma}'}\ , \tag{16b}$$

and the dimension of the relevant space R_0 can be reduced by introducing $S^{\pi}_{d}=\sum_i S^{\pi}_{i,i+d}$, and $S^{\eta}_{d}=\sum_i S^{\eta}_{i,i+d}$.

So the band gap E_g includes two parts: mean-field gap 2Δ and correlation gap E_g^{corr},

$$E_g^{\text{corr}}=2\varepsilon^{\text{corr}}(k=\pi/2)\ . \tag{17}$$

The calculation of the correlation gap needs the functions $E_{ll'}$, $\tilde{E}_{ll'}$, and $R_{ll'}$. Having the aid of the correlation functions

$$P_{ij}\equiv\langle 0|c^{\dagger}_{i\sigma}c_{j\sigma}|0\rangle \quad\text{and}\quad Q_{ij}\equiv\langle 0|c_{i\sigma}c^{\dagger}_{j\sigma}|0\rangle\ ,$$

$|0\rangle$ is the ground state of mean-field Hamiltonian of Eq. (6), we obtain

$$E_{ll'}\equiv(c_{l\sigma}|\hat{h}^{e}_{0}c_{l'\sigma})=\sum_i\left[P_{li+1}P_{il'}+P_{li}P_{i+1l'}-(-1)^{i}\Delta P_{li}P_{il'}\right]\ , \tag{18}$$

$$\tilde{E}_{ll'}\equiv(c^{\dagger}_{l\sigma}|\hat{h}^{e}_{0}c^{\dagger}_{l'\sigma})=\sum_i\left[-Q_{li}Q_{i+1l'}-Q_{li+1}Q_{il'}+(-1)^{i}\Delta Q_{li}Q_{il'}\right]\ , \tag{19}$$

and for $k=\pi/2$,

$$R_{ll'}=\begin{cases}(-1)^{l'/2-l/2}, & l,l' \text{ are even}\\ 0 & \text{otherwise}\ ,\end{cases} \tag{20}$$

$R_{ll'}(k)$ is defined by $R_{ll'}(k)/N\equiv(A^{\dagger}_{k\sigma}|a^{\dagger}_{l\sigma}a_{l'\sigma}A^{\dagger}_{k\sigma})$.

By using the wave function we have obtained, the correlation functions can be easily obtained,

$$P_{n,n+2m}=\frac{1}{2\pi}\int_{-\pi/2}^{\pi/2}dk\, e^{i2mk}\left[1-(-1)^{n}\frac{\Delta}{E_k}\right]\ , \tag{21a}$$

$$P_{n,n+2m-1}=-\frac{1}{2\pi}\int_{-\pi/2}^{\pi/2}dk\, e^{i(2m-1)k}\frac{\epsilon_k}{E_k}\ . \tag{21b}$$

It should be noted that $P_{n,n+2m}$ depends on the parity of n, because the ground state is the CDW, the average charge density is different according to the parity of n, even or odd.

Since the function $P_{n,n+m}$ decreases as $\exp(-|m|\Delta)$ for large m, we truncate the series by assuming that $P_{ij}=0$ for $|i-j|\geq 5$, i.e., only the following functions are considered:

$$P_{nn}=\tfrac{1}{2}-(-1)^{n}\frac{\Delta}{\pi\sqrt{4+\Delta^2}}K\left[\frac{2}{\sqrt{4+\Delta^2}}\right]\ , \tag{22a}$$

$$P_{n,n+1}=\frac{1}{2\pi}\left[\sqrt{4+\Delta^2}E\left[\frac{2}{\sqrt{4+\Delta^2}}\right]-\frac{\Delta^2}{\sqrt{4+\Delta^2}}K\left[\frac{2}{\sqrt{4+\Delta^2}}\right]\right]\ , \tag{22b}$$

$$P_{n,n+2}=-(-1)^{n}\frac{1}{2\pi}\left[\Delta\sqrt{4+\Delta^2}E\left[\frac{2}{\sqrt{4+\Delta^2}}\right]-\frac{\Delta^3+2\Delta}{\sqrt{4+\Delta^2}}K\left[\frac{2}{\sqrt{4+\Delta^2}}\right]\right]\ , \tag{22c}$$

$$P_{n,n+3}=\frac{3}{2\sqrt{\Delta^2+4}}\left[F\left[\tfrac{1}{2},\tfrac{1}{2};3;\frac{4}{4+\Delta^2}\right]-F\left[\tfrac{1}{2},\tfrac{1}{2};2;\frac{4}{4+\Delta^2}\right]\right]\ , \tag{22d}$$

$$P_{n,n+4}=-(-1)^{n}\frac{\Delta}{\pi\sqrt{\Delta^2+4}}\left[\frac{3\pi}{2}F\left[\tfrac{1}{2},\tfrac{1}{2};3;\frac{4}{4+\Delta^2}\right]-2\pi F\left[\tfrac{1}{2},\tfrac{1}{2};2;\frac{4}{4+\Delta^2}\right]+K\left[\frac{2}{\sqrt{4+\Delta^2}}\right]\right]\ , \tag{22e}$$

where $E(x)$ is the second-kind complete elliptic integrals, $F(\alpha,\beta;\gamma;z)$ is the hypergeometric function. We confine the dimension of the relevant space to 20, i.e., only $S_d^{\pi(\eta)}$ $(d=0,1,\ldots,19)$ gives nonzero contribution to the band gap.

Figures 1 and 2 illustrate the band gap and the correlation gap as the functions of the Hubbard parameter u with *e-p* coupling $s=0.75$. The three lines in Fig. 1 correspond to the projection technique, MFT, and the second-order perturbation, respectively, and the dimerization of the ground state is fixed in the MFT value. It is seen that the correlation reduces the mean-field band gap and this correction becomes more obvious when the Hubbard interaction increases. The perturbation method also indi-

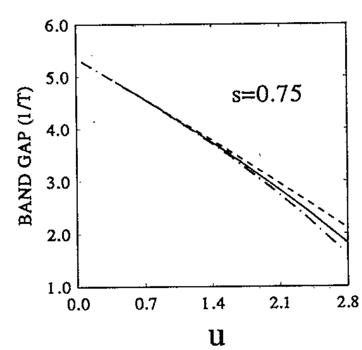

FIG. 1. Band gap E_g as a function of Hubbard parameter u with *e-p* coupling $s=0.75$. Solid line is the result achieved by the projection technique. Short-dashed line and dot-dashed line indicate the mean field and second-order perturbation in Ref. 8, respectively.

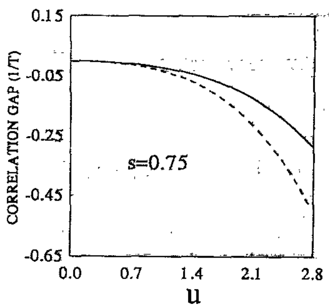

FIG. 2. Correlation gap E_g^{corr} as a function of Hubbard parameter u with e-p coupling $s=0.75$. Solid and dashed lines correspond to projection technique and second-order perturbation theory, respectively.

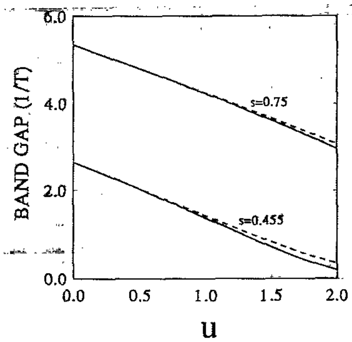

FIG. 3. Band gap E_g as a function of Hubbard parameter u for different e-p coupling $s=0.75$ and 0.455. Solid lines are the results achieved by the projection technique and short-dashed lines indicate the mean-field results.

cates that the Hubbard interaction narrows the band gap. When u is small, the difference between these two approaches should be very small, since the perturbation theory is accurate when u is going to zero. However, when u increases, the difference becomes large. It should be emphasized that in projection technique, the calculation is "self-consistent" and the interaction is "renormalized"; this can be realized if we note that the Hubbard parameter u also appears in the denominator of the expressions of the correlation gap.[6] Therefore this approach is also valid when the strength of the e-e interaction becomes significant, and the results obtained by the projection technique are more reliable when u is not small.

For $s=0.75$, the relatively strong e-p coupling, the further decrease of the band gap due to the correlation is about 9% of the one obtained from MFT at $u=2.8$. This smallness of the correlation effect in the MX complex is easy to understand. Strong e-p coupling leads to large amplitude of CDW and the charge distribution is nearly localized (the odd sites are doubly occupied and the even sites are empty), in fact, in the completely localized limit, where the electron hopping is neglected, the Hartree-Fock approximation is rigorous. Naturally, the bigger correlation effect is expected in the case with weaker charge disproportionation. This is confirmed by the comparison between different e-p coupling in Fig. 3. At $u=2.0$, among the total reduction of the band gap by the Hubbard interaction, the correlation part accounts for 5% for $s=0.75$ and 7% for $s=0.455$. We can also compare this correction magnitude with that in polyacetylene. To make this comparison meaningful, we measure the e-p by another dimensionless constant λ_2 defined in Ref. 11 and $\lambda_2=2s/\pi$, so $s=0.455$ corresponds to $\lambda_2=0.29$. In polyacetylene, for $\lambda=0.29$, the correlation increases the gap parameter Δ about 25% at $U/4t_0=0.5$,[12] and this magnitude is much larger than that in the MX complex. The comparison for smaller λ_2 is not made, since for very weak e-p coupling, the CDW is unstable with respect to spin-density wave in the presence of Hubbard interaction.[2,13]

It is very interesting to note that the electron correlation narrows the band gap; it is contrary to the situation in polyacetylene. In the MX complex, when the e-e interaction is absent, the ground state is the CDW and a gap is opened due to the X-sublattice dimerization caused by the site-diagonal e-p coupling. Since the charges are different between the odd- and even-numbered M atom in the CDW state, the double occupation arises. But, in polyacetylene, the ground state is BOW, and there is no double occupation. Within MFT, the Hubbard repulsion only affects the double occupation, and reduces the dimerization and the band gap in the MX complex; however, it has no effect on polyacetylene, so the correlation effect is more manifest in polyacetyelene. When the correlation is included, the *loss* of correlation energy is dominant in polyacetylene; on the other hand, the *gain* of polarization energy is dominant in the MX complex. This is connected with the difference of the charge distributions between these materials. For BOW, the charge distribution varies from bond to bond, not from site to site; but for CDW, the charge varies from site to site, not from bond to bond. These different charge distributions in the ground states lead to the different effects of the electron correlation, which enhances the band gap of polyacetylene and reduces the band gap in the MX complex.

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