PHYSICAL REVIEW B VOLUME 61, NUMBER 24 15 JUNE 2000-II

GW quasiparticle band structure of YH_3

Takashi Miyake and Ferdi Aryasetiawan
Joint Research Center for Atom Technology, Angstrom Technology Partnership, 1-1-4 Higashi, Tsukuba, Ibaraki 305-0046, Japan

Hiori Kino
Institute for Solid State Physics, University of Tokyo, Roppongi, Minato-ku, Tokyo 106-8666, Japan

Kiyoyuki Terakura
Joint Research Center for Atom Technology, National Institute for Advanced Interdisciplinary Research, 1-1-4 Higashi, Tsukuba, Ibaraki 305-8562, Japan
and CREST, Japan Science and Technology Corporation, Kawaguchi, Saitama 332-0012, Japan

(Received 13 September 1999; revised manuscript received 24 January 2000)

We present an *ab initio* calculation of YH_3 using the GW approximation (GWA). Although a density-functional calculation incorrectly gives a metallic state unless we assume a very complicated structure, the self-energy correction with the GWA removes the band overlap, and reproduces insulating behavior. Hence, the failure of the density-functional calculation can be attributed to an electronic origin. The role of the self-energy is to raise the unoccupied Y $4d$ band rather than to decrease the bandwidth of the occupied H $1s$ band.

I. INTRODUCTION

Among continuous researches on metal hydrides for decades, the recent experiment by Huiberts *et al.*[1] on yttrium and lanthanum hydrides (YH_x and LaH_x) occupies a special place in the sense that hydrogen induces dramatic changes in the electronic and optical properties. Yttrium and lanthanum can absorb a large quantity of hydrogen. YH_2 and LaH_2 are known to be metallic but, when the hydrogen concentration x is increased, the materials show a metal-insulator transition at around $x=2.8$ and turn transparent. Unlike other metal-insulator transitions, the transition in yttrium and lanthanum hydrides is reversible and it occurs in the visible range, thereby making them attractive for application as optical switches. Consequently, these materials have drawn much attention among both experimentalists and theorists. Other experiments followed for deeper understanding of the phenomenon,[2,3] and now it is known that the transition is common in a wide range of lanthanide hydrides.[4] There is also evidence that by choosing suitable rare-earth elements, the transition can be made very quick, which is desirable in optical switching applications.

The electronic structure of yttrium and lanthanide hydrides is unfortunately poorly understood. Theoretical work on these materials has followed several lines. Band-structure calculations based on the local density approximation (LDA) of density-functional theory predict YH_3 and LaH_3 to be metals, with a band overlap of about 1 eV, instead of the experimentally observed semiconductors.[5,6] In the case of yttrium hydride, the transition is accompanied by a structural transformation from cubic to hexagonal. The electronic structure for several possible structures, such as the LaF_3 and HoD_3 structures, have also been calculated but the band structures still show metallic behavior. This stimulated further analysis.

The discrepancy could be due to a structure effect. There may be a more complicated structure which is more stable and insulating. Kelly *et al.* conducted a study along this line. Starting from the HoD_3 structure, they found a broken symmetry structure, which is slightly more stable than the HoD_3 structure and has a LDA gap of 0.75 eV.[7] However, there is controversy as to whether the structure is consistent with neutron diffraction data.[8,9] Actually, the relaxation energy is so small (less than 0.1 eV per Y_6H_{18}) that thermal and quantum fluctuation could easily smear out the distortion. In addition, it is known that the gradient correction to the LDA is significant for systems including hydrogen. A more careful analysis is thus required. Another difficulty with the explanation based on the broken symmetry structure is that the transition of lanthanum hydrides occurs without structural transformation: The system remains cubic during the transition.[3] This suggests that the transition is not connected with the structure and has an electronic origin.

Considering these observations, some theories, as we shall describe later, have been proposed that claim that electron correlation at the hydrogen site is crucial to open a gap.[10,11] However, these arguments are based on simple models. To look into the many-body effects beyond the LDA, further study with an *ab initio* scheme is desirable. From this point of view, in the present work, we calculate the quasiparticle band structure with the GW approximation (GWA).[13] We shall show that the self-energy correction is large enough to open a gap, although band narrowing is not observed. In the light of our results, we discuss possible mechanisms that are likely to explain the electronic structure of the yttrium and lanthanide hydrides.

II. METHOD

In the GWA,[12,13] the self-energy is expressed as

$$\Sigma(\mathbf{r},\mathbf{r}';\omega)=\frac{i}{2\pi}\int d\omega\, G(\mathbf{r},\mathbf{r}';\omega+\omega')W(\mathbf{r},\mathbf{r}';\omega'), \quad (1)$$

$$W(\mathbf{r},\mathbf{r}';\omega)=\int d^3r''\epsilon^{-1}(\mathbf{r},\mathbf{r}';\omega)v(r''-r'). \qquad (2)$$

In practical calculations, the Green function G is constructed from the LDA wave functions $\{\psi^{\mathrm{LDA}}\}$ and eigenvalues $\{\epsilon^{\mathrm{LDA}}\}$. This Green function is used to calculate the inverse dielectric function ϵ^{-1} within the random phase approximation (RPA). The quasiparticle energy $E^{\mathrm{QP}}_{\mathbf{k}n}$ is then calculated from the self-energy as

$$E^{\mathrm{QP}}_{\mathbf{k}n}=\epsilon^{\mathrm{LDA}}_{\mathbf{k}n}+Z_{\mathbf{k}n}\langle\psi^{\mathrm{LDA}}_{\mathbf{k}n}|\Sigma(\epsilon^{\mathrm{LDA}}_{\mathbf{k}n})-V^{\mathrm{LDA}}_{\mathrm{xc}}|\psi^{\mathrm{LDA}}_{\mathbf{k}n}\rangle, \qquad (3)$$

where $V^{\mathrm{LDA}}_{\mathrm{xc}}$ is the LDA exchange-correlation potential, and $Z_{\mathbf{k}n}\equiv[1-\partial\Sigma_{\mathbf{k}n}(\omega)/\partial\omega|_{\omega=\epsilon^{\mathrm{LDA}}_{\mathbf{k}n}}]^{-1}$ is the renormalization factor.

In addition to this non-self-consistent procedure, we have also employed a semi-self-consistent procedure in calculating the self-energy.[14] We start from the LDA Hamiltonian and calculate the self-energy correction. The main effect of the self-energy correction is to raise the conduction band which is primarily of Y $4d$ character. In the next iteration, we then introduce a potential of the form $\alpha|Y_{4d}\rangle\langle Y_{4d}|$ with α chosen such that the shift due to the self-energy correction from the previous iteration is reproduced. The wave functions and the eigenvalues for the shifted potential are used to evaluate new G and ϵ, from which the new self-energy is calculated. This process is repeated until the self-energy correction does not change the value of the gap.

Our calculation is based on the linear-muffin-tin-orbital (LMTO) method within the atomic-sphere approximation.[15] The atomic-sphere radii used in the present work are the same as those in Ref. 5. The response function and the self-energy are expressed as the products of wave functions. In order to reduce the computational task, we apply the product basis method proposed in Ref. 16. Typically 50–100 product basis functions are needed per atom. The band structure is calculated with an $8\times8\times8$ $\mathbf{k}$-point mesh for the $\mathrm{BiF_3}$ structure. For the $\mathrm{LaF_3}$ structure with a larger unit cell, we use a $6\times6\times4$ mesh. The frequency dependence of the dielectric function is treated fully without resorting to simplifications such as the plasmon-pole approximation. Details of the technique are found in Ref. 17.

III. BAND STRUCTURE

A. $\mathrm{BiF_3}$ structure

We begin with the calculation of the $\mathrm{BiF_3}$ structure. In this structure, Y atoms form a fcc structure. Two hydrogens (per one Y atom) are at the tetrahedral interstitial site, and one occupies the octahedral interstitial site.

In Fig. 1 the LDA density of states is shown. The valence band is predominantly hydrogen $1s$ with a mixture of Y ($5s$, $5p$, and $4d$) whereas the conduction band is dominated by Y $4d$ with some mixing of hydrogen $1s$. The hydrogen band is very broad with a width extending to 10 eV, which is much larger than the estimated value of U of 2 eV.[11]

In Fig. 2(a), we show the band structures obtained by the LDA and the GWA. The GW self-energy correction does not change the valence band very much. (The band is raised up slightly as a whole. However, this should be cancelled out if the Fermi energy is adjusted to conserve particle number.)

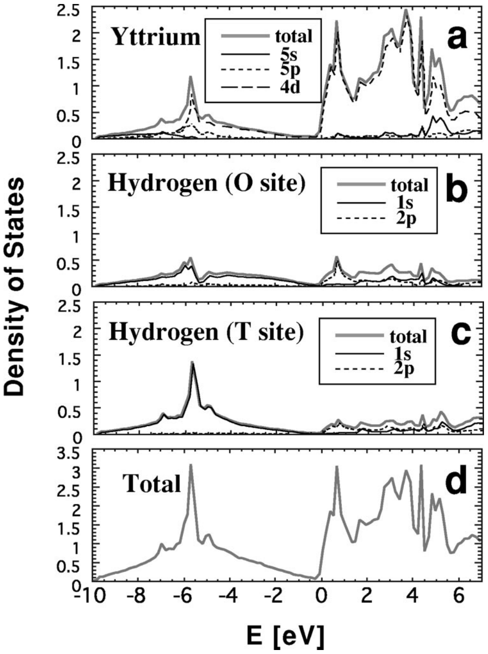

FIG. 1. The LDA density of states (DOS) of $\mathrm{YH_3}$. The DOS is projected on (a) yttrium and (b) hydrogen at the octahedral site, and (c) hydrogen at the tetrahedral site. The number of hydrogens at the octahedral (tetrahedral) site is 1 (2) per formula unit. The solid line, short dashed line, and long dashed line are the contributions from the s, p, and d orbitals, respectively. The gray line is the sum of the three. (d) Total density of states. The energy is measured with respect to the Fermi energy.

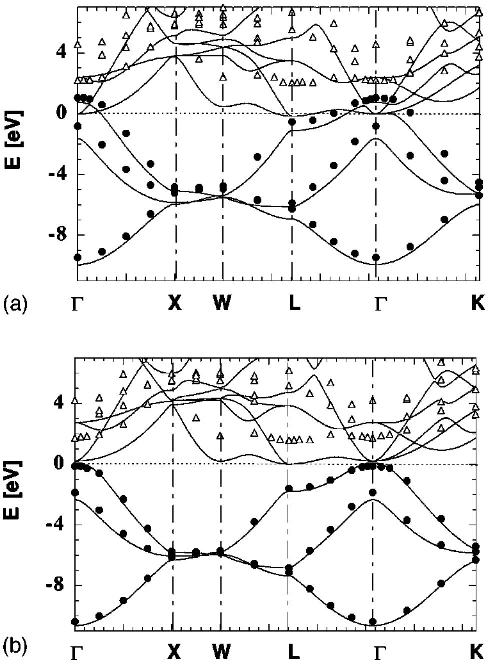

FIG. 2. (a) The GW quasiparticle band structure of $\mathrm{YH_3}$ with the $\mathrm{BiF_3}$ structure. The filled circles (empty triangles) denote the valence (conduction) bands. The solid line represents the LDA band. (b) The same as (a) but the LDA Y $4d$ bands are shifted up by 1.2 eV. The dotted horizontal line denotes the location of the Fermi level of the LDA band.

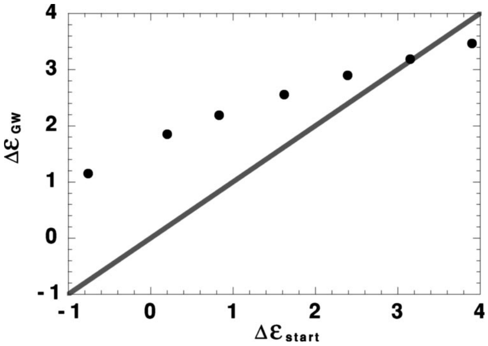

FIG. 3. The GW gap ($\Delta\epsilon_{GW}$) against the gap of the starting Hamiltonian ($\Delta\epsilon_{\rm start}$) in which the Y 4$d$ band is shifted up compared to the LDA bands. The solid line is $\Delta\epsilon_{GW}=\Delta\epsilon_{\rm start}$, plotted for comparison.

The self-energy correction is much larger for the conduction bands. It shifts up the bands by about 2 eV.

The LDA band structure shows a band overlap at the Γ point[5] with a magnitude of, in our estimation, 0.8 eV. The highest occupied state is triply degenerate and of Y 4d character. It shifts up by 2.2 eV when we add the self-energy correction. On the other hand, the lowest unoccupied state, with H 1s character, changes by only 0.3 eV. As a result, the order of the two states is reversed, and consequently the quasiparticle band becomes insulating with a gap at the Γ point of 1.2 eV. In the present calculation, the conduction band minimum is located at the L point, although the energy difference between this point and the lowest unoccupied state at the Γ point is small. (As we shall see later, and also in Ref. 5, the position of the minimum gap depends on the structure. It is thus difficult to distinguish whether the gap of the real material is direct or indirect.)

Considering the rather poor starting Hamiltonian with a band overlap of almost 1 eV, this one-iteration result is very reasonable. Most GW calculations on real materials are performed with one iteration. In those materials where the LDA Hamiltonian already gives a reasonable band structure, one-iteration calculations have turned out to give very good results. In this respect, it is interesting to bring up a question about the starting Hamiltonian. We obtained an insulating state starting from a metallic state. This means that the charge density given by the LDA is different from the real one. The screening effect will be overestimated, and so the self-energy correction may be quantitatively incorrect. A simple and reasonable way to overcome this difficulty is to shift the bands so that the starting Hamiltonian has a small gap. We shifted the Y 4d LMTO orbital after the self-consistent LDA calculation, and did an extra LDA calculation for one iteration. Starting from this *shifted* Hamiltonian, we estimated the self-energy correction, and added the correction to the *unshifted* LDA eigenvalues. This procedure gives a quasiparticle band shown in Fig. 2(b). The overall picture is the same as Fig. 2(a). The valence band is unchanged, while the conduction band is raised. The gap is larger than the unshifted one because of less screening, and is estimated to be 1.9 eV.

What happens then if we shift the Y 4d band further? In Fig. 3, we plot the GW gap against the gap of the shifted Hamiltonian from which the self-energy is calculated. (Here a negative gap means band overlap.) As we increase the shift, the GW gap increases monotonically. The self-energy correction, however, decreases, and the GW gap becomes smaller when we start from a very large gap. The two gaps match when they are 3.2 eV. The experimental gap is 1.8 eV. (Note, however, that the structure used in the present calculation is different from the experimental one, whose details are not known.)

This simplified self-consistent procedure turned out to overestimate the gap somewhat, similarly to the case of NiO.[14] On the other hand, according to a recent calculation for Si, a fully self-consistent GW calculation using the dressed Green function also results in a too large gap.[18] In the fully self-consistent procedure, the response function does not have a clear physical meaning either. Unlike $P=-iG_0G_0$, with G_0 given by the LDA Green function, which is the response function of the noninteracting system described within the LDA, the quantity $P=-iGG$, with G given by the GW Green function, does not in general correspond to some non-interacting system anymore. Indeed, this leads to the disappearance of the plasmon satellite, which is unphysical.[19]

An alternative and physically sound scheme needs to be developed for the quantitative description of systems for which the LDA does not give a good starting point. It seems that a fruitful procedure is the ‘‘best G best W’’ approach. The definition of the best G is ambiguous but the idea is to use the calculated self-energy to construct a better starting Hamiltonian. One can imagine a sort of self-consistent process when the one-particle spectrum is not significantly altered by the self-energy. We then take the corresponding Hamiltonian as the final starting Hamiltonian for a one-iteration calculation. The feasibility of such a scheme is illustrated in the present work, albeit in a crude way.

Going back to our results, we find that the valence band is insensitive to the self-energy correction. For the unshifted/shifted case shown in Figs. 2(a)/2(b), the quasiparticle band width is 10.5/10.2 eV compared to that of the LDA, 10.7/10.7 eV. The GWA is expected to narrow bands whose widths are overestimated by the LDA.[20,14] It is therefore unlikely that the mechanism of gap opening is due to band narrowing. The renormalization factor Z is typically 0.8–0.9, and is even larger than those of semiconductors. These facts suggest that electron correlation is not very strong in this system, as sometimes assumed.

B. LaF_3 structure

To investigate whether the semiconducting state is structure dependent, we now perform a calculation for the LaF_3 structure. In this structure, Y forms a hcp lattice. Among three hydrogens per one Y atom, one is on the metal plane, and the other two occupy the tetrahedral site which is between two metal planes.

In Fig. 4, we show the band structure. The LDA band is semimetallic with a band overlap of 1.4 eV. As is the case in the previous section, the conduction band is shifted up by about 2 eV by the self-energy. The valence band does not change significantly in either width or location of the center. When we look at the detail, however, the self-energy correction is highly state dependent. For example, the shape of the

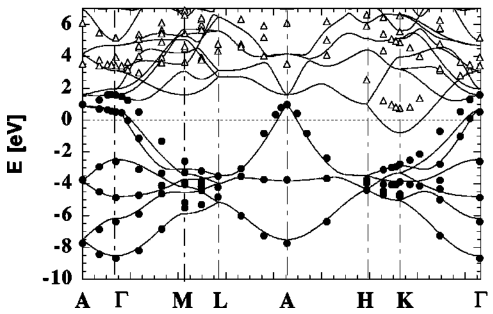

FIG. 4. The quasiparticle band structure for the LaF$_3$ structure. Filled circles (empty triangles) denote the valence (conduction) bands. Solid line represents the LDA band. The dotted horizontal line denotes the location of the Fermi level of the LDA band.

band is modified in the occupied part of the H-K and M-L lines. We have analyzed the character of the states, and found that the self-energy correction raises the energy by about 1 eV when the state is of tetrahedral hydrogen character, while it shifts the energy down when the state has little tetrahedral hydrogen component. As for the hole pocket, one of the two bands at $\boldsymbol{\Gamma}$ is of tetrahedral hydrogen character, and is shifted up by about 1 eV. The net contribution of the self-energy correction decreases the band overlap from 1.4 eV (LDA) to 0.8 eV (GWA).

The decrease of band overlap changes the charge density of the ground state. This, as in the case of the BiF$_3$ structure, requires adjusting the starting Hamiltonian so that the initial band structure is close to the real one. We shifted the bands just enough to open up a small gap and used this shifted Hamiltonian to estimate the self-energy. This results in an insulating state with a gap between the $\boldsymbol{\Gamma}$ point (valence state) and the $\mathbf{K}$ point (conduction state) of 1.1 eV. Following the same simplified self-consistent procedure as in the fcc case, we would obtain a curve similar to the one shown in Fig. 3. This result suggests that the band gap is controlled mostly by the electronic interaction rather than by the crystal structure.

IV. OPTICAL ABSORPTION AND LOSS SPECTRA

In addition to the quasiparticle energies, we have also calculated the following dielectric function:

$$\epsilon(\mathbf{q},\omega)=\frac{1}{V}\int d\mathbf{r}\,d\mathbf{r}'\,e^{-i\mathbf{q}\cdot\mathbf{r}}\epsilon(\mathbf{r},\mathbf{r}';\omega)e^{i\mathbf{q}\cdot\mathbf{r}'}, \tag{4}$$

with small $\mathbf{q}$. The imaginary part of $\epsilon(\mathbf{q},\omega)$ gives the optical absorption, and the imaginary part of $\epsilon^{-1}(\mathbf{q},\omega)$ gives the energy loss spectrum. The calculation is done with a $12\times12\times12$ $\mathbf{k}$-point mesh for the BiF$_3$ structure. The optical property is obtained in the limit of $\mathbf{q}\rightarrow0$. However, our code works for a finite $\mathbf{q}$ only, so we use the smallest $\mathbf{q}$ vector $(\frac{1}{12},\frac{1}{12},\frac{1}{12})(2\pi/a)$ as a substitute for $\mathbf{q}=(0,0,0)$.

In Fig. 5(a) the optical absorption spectra from the two methods are compared. In the LDA case, the LDA wave function and eigenvalues are used. In the shifted case, on the other hand, the Y $4d$ band is shifted in the same way as described in Sec. II so that the gap is the same as the experimental one. The wave function and eigenvalues for this modified LDA potential are used to calculate the spectra. In the LDA the system is metallic and the spectrum accordingly shows a Drude peak at low energy. This is in contrast to the spectrum calculated using the quasiparticle energies, which shows a gap. Experimental spectra would be valuable in assessing the quality of the different band structures. The spectrum shows a multiple peak structure at around 5 eV and additional peaks at about 12 eV and 19 eV.

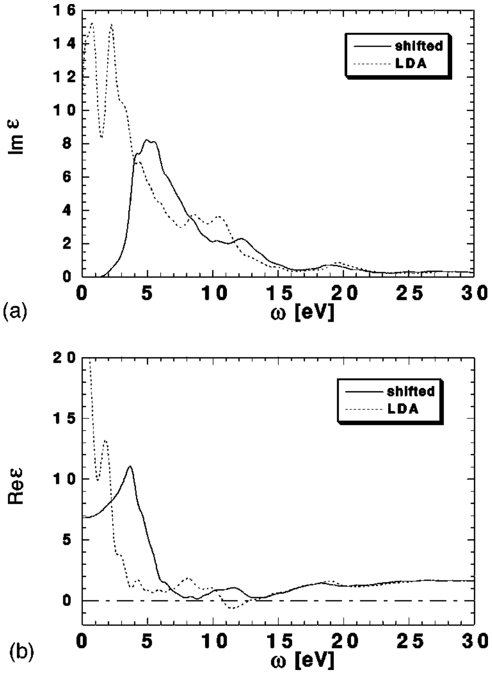

FIG. 5. The dielectric function function $\epsilon(\mathbf{q},\omega)$ at $\mathbf{q}=(\frac{1}{12},\frac{1}{12},\frac{1}{12})(2\pi/a)$ for the BiF$_3$ structure. (a) The imaginary part and (b) the real part.

The loss spectra, on the other hand, are not sensitive to the one-particle energies as can be seen in Fig. 6(a). This is because the main excitation is dominated by the plasmon whose energy is large and it is essentially fixed by the f sum rule. The peak around 15 eV may be identified as a plasmon excitation. This energy agrees very well with an estimate based on the electron gas formula. The two secondary peaks at 11 eV and 20 eV may be traced back to the two peaks in Im ϵ at 12 and 19 eV, respectively, described in the previous paragraph. No experimental data are available so far for comparison of either the optical absorption or the energy loss spectra.

It is interesting to compare the real part of the dielectric function calculated in the LDA and in the self-energy-corrected LDA [Fig. 6(b)]. As can be understood from Eq. (2), Re$(1/\epsilon)$ characterizes the strength of the screening. We clearly see a significant difference in the values of Re$(1/\epsilon)$ at low frequencies. The LDA inverse dielectric function is small since the system is metallic, whereas the shifted LDA one is considerably larger since the corresponding system is an insulator. The small value of the LDA inverse dielectric function, which implies too much screening, is probably responsible for the insufficient self-energy correction when only one iteration is performed. Redefining the starting Hamiltonian by taking into account the self-energy correction from the first iteration should give a more realistic band structure. This results in a larger inverse dielectric function

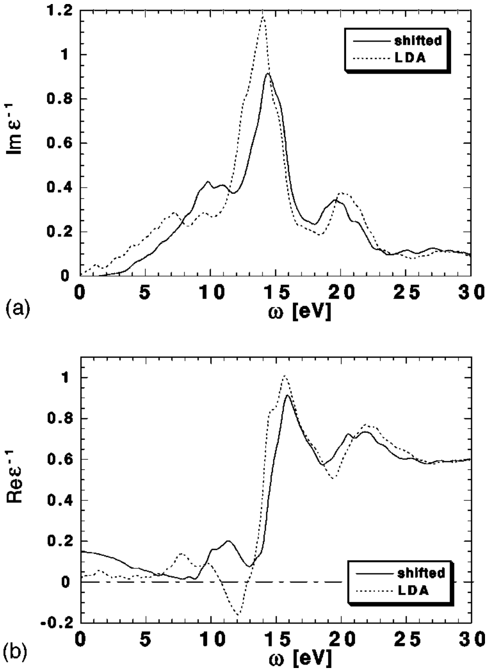

FIG. 6. The inverse dielectric function $1/\epsilon(\mathbf{q},\omega)$ at $\mathbf{q}=(\frac{1}{12},\frac{1}{12},\frac{1}{12})(2\pi/a)$ for the BiF_3 structure. (a) The imaginary part and (b) the real part.

and the difference in the screening enhances the opening up of the band gap in subsequent iterations. The situation is similar to the NiO case[14] and in general we expect to observe a similar behavior in cases where the LDA band structures deviate a great deal from the true quasiparticle ones. Thus, for a one-iteration *GW* scheme to work successfully, it seems important that the starting one-particle spectrum should be as close as possible to the true quasiparticle one.

V. COMPARISON WITH OTHER THEORIES

There are a few theories proposed in the literature to explain the semiconducting nature of the yttrium and lanthanide trihydrides based on electron correlation. Now we will discuss them in detail. Ng *et al.* studied the correlation problem in metal hydrides using a model Hamiltonian.[10] The Hamiltonian is divided into three terms: the hydrogen part, the yttrium/lanthanum part, and a mixing term. Since the hydrogen band is fully occupied, the hydrogen should be in the H^- state. A single H^- ion is a bound state and they assume that the ionic picture is valid. They studied the effect of correlations on the H^- bandwidth using the correlated Chandrasekhar wave function and arrived at an expression for the hopping integral between neighboring hydrogens. In addition, they also included the effect of the crystal field which was found to significantly reduce the hopping integral, by about 60%. A feature of the model is the constraint that the total occupation number of the hydrogen site is always greater than 1. This corresponds physically to the fact that the two electrons in the H^- ion have very different energies; the inner one is tightly bound whereas the outer one is mobile. In other words, the model prevents the presence of two holes on the hydrogen site. The parameters in the model are determined by a combination of microscopic calculations for the hopping integrals between the hydrogen sites and LDA calculations for the hybridization between La and H. The model is then solved using the Gutzwiller method, predicting LaH_2 to be metallic and LaH_3 to be an insulator. The essence of their result is that the opening of the band gap is caused by the reduction in the hydrogen bandwidth due to correlations in H^- ions.

Another related theory was proposed by Eder *et al.*[11] The model is based on the observation that the radius of the hydrogen is very sensitive to the occupation number. Thus for a neutral hydrogen the radius is 0.26 Å whereas the radius of H^- is 1.54 Å. This strong dependence on the occupation number is incorporated into the model by having a novel hopping integral which depends on the occupation number of the hydrogen. This results in the formation of a local singlet-like bound state involving one electron on H and one on the neighboring metal orbitals. Already, at the mean-field level, the occupation-dependent hopping integral introduces a significant correction to the potential at the H site, lowering the hydrogen band, which in turn opens up a gap. This model and the previous model have something in common in that both treat the hydrogens as impurities in the background of the yttrium/lanthanide metals. The mechanism for gap opening, however, is quite different. In the previous model, the gap opening is a result of hydrogen band narrowing, whereas in the model of Eder *et al.* the gap opening is due to a shift in the potential at the hydrogen site (scissor operator) retaining the broad hydrogen band.

If we now put in perspective the theories discussed above in the light of our results, we could say the following. In contrast to the LDA results, our *GW* calculations show that it is not necessary to have a broken symmetry structure to open up the gap. Both the calculations with cubic and hexagonal structures produce the band gap and thus the gap is of electronic origin rather than structural. Regarding the hydrogen band, there is no indication of band narrowing as suggested by the model of Ng *et al.* Such a band narrowing in the GWA must come from the long-range screening, which should be at least partially captured by the RPA. We also observe that the calculated renormalization factor (Z factor) for the hydrogen states, $Z=0.8$–0.9, is actually larger than in normal semiconductors. This large value means that the hydrogens participate little in plasmon excitations associated with long-range screening. The renormalization factor usually indicates the strength of correlations and such a large value suggests that correlations beyond the LDA are not as large as anticipated. This value is to be compared with that in Ni ($Z=0.5$) or Gd ($Z=0.3$). Thus we could say that, if it is true that the hydrogen band is narrowed, this must be due to short-range correlations which are not accounted for in the GWA. We cannot therefore rule out the model of Ng *et al.* although our results show that the mechanism of gap opening is rather similar to that in normal semiconductors, where the upward shift of the conduction band results from state-dependent self-energy. In this respect, the model of Eder *et al.* conforms better with our results, although in their model, the gap opening is affected by shifting down the hydrogen band whereas in our case the gap opening is due to the shifting up of the conduction band.

It is pointed out in the literature that LDA calculation of

YH_3 produces a large band overlap of almost 1 eV, which means that a correction of about 3 eV is needed since the experimental gap is 1.8 eV. This then is taken to be an indication of strong correlations. On the other hand, the LDA is known to underestimate, and sometimes collapse, a band gap so that a poor LDA result in this case does not necessarily imply strong correlations. Moreover, the hydrogen bandwidth is much larger than the estimated value of the Hubbard U (2 eV),[11] so that the usual criterion of strong correlation is far from satisfied. Our results suggest that YH_3 is a normal semiconductor. The fact that a one-iteration GW calculation does not immediately give the correct gap is likely due to the poor starting LDA Hamiltonian. When a simplified self-consistent procedure is applied, the gap becomes larger although the final self-consistent gap is too large. This crude procedure, however, requires some refinements. One necessary requirement is to have a self-consistent one-particle starting Hamiltonian, and work along this line is now in progress.

VI. CONCLUDING REMARKS

We have calculated the quasiparticle band structure of YH_3 within the GW approximation. Neither band narrowing nor strong renormalization is observed. This suggests that correlations beyond the LDA are not as strong as sometimes assumed. The main role of the self-energy correction is just raising the conduction band, as in semiconductors such as Si. This shift is large enough to remove the band overlap observed in the LDA. Therefore, the discrepancy between the LDA calculation and experiments can be explained in terms of an electronic origin rather than a structural origin. The large discrepancy between the LDA and the experimental results could well be due to the poor performance of the LDA in the band gap rather than to strong correlations. When an attempt is made to improve the starting Hamiltonian in the GW calculations by a simplified self-consistent procedure, the gap indeed becomes larger, although for more quantitative discussion of the gap, a more careful analysis is required on self-consistency. In this sense, our results suggest that YH_3 is a normal semiconductor like Si. Our results partially support the theoretical model proposed by Eder *et al.*, but a photoemission experiment is crucial in resolving the electronic structure of metal hydrides.

ACKNOWLEDGMENTS

This work is partly supported by the New Energy and Industrial Technology Development Organization (NEDO), and also by the Research for the Future Program of the Japan Society for the Promotion of Science.

---

[1] J. N. Huiberts, R. Griessen, J. H. Rector, R. J. Wijngaarden, J. P. Dekker, D. G. de Groot, and N. J. Koeman, Nature (London) **380**, 231 (1996).

[2] J. N. Huiberts, R. Griessen, R. J. Wijngaarden, M. Kremers, and C. Van Haesendonck, Phys. Rev. Lett. **79**, 3724 (1997).

[3] M. Kremers, N. J. Koeman, R. Griessen, P. H. L. Notten, R. Tolboom, P. J. Kelly, and P. A. Duine, Phys. Rev. B **57**, 4943 (1998).

[4] P. van der Sluis, M. Ouwerkerk, and P. A. Duine, Appl. Phys. Lett. **70**, 3356 (1997).

[5] J. P. Dekker, J. van Ek, A. Lodder, and J. N. Huiberts, J. Phys.: Condens. Matter **5**, 4805 (1993).

[6] Y. Wang and M. Y. Chou, Phys. Rev. Lett. **71**, 1226 (1993); Phys. Rev. B **51**, 7500 (1995).

[7] P. J. Kelly, J. P. Dekker, and R. Stumpf, Phys. Rev. Lett. **78**, 1315 (1997).

[8] T. J. Udovic, Q. Huang, and J. J. Rush, Phys. Rev. Lett. **79**, 2920 (1997).

[9] P. J. Kelly, J. P. Dekker, and R. Stumpf, Phys. Rev. Lett. **79**, 2921 (1997).

[10] K. K. Ng, F. C. Zhang, V. I. Anisimov, and T. M. Rice, Phys. Rev. Lett. **78**, 1311 (1997).

[11] R. Eder, H. F. Pen, and G. A. Sawatzky, Phys. Rev. B **56**, 10 115 (1997).

[12] L. Hedin, Phys. Rev. **139**, A796 (1965).

[13] L. Hedin and S. Lundqvist, in *Solid State Physics: Advances in Research and Applications*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1969), Vol. 23, p. 1.

[14] F. Aryasetiawan and O. Gunnarsson, Phys. Rev. Lett. **74**, 3221 (1995).

[15] O. K. Anderson, Phys. Rev. B **12**, 3060 (1975).

[16] F. Aryasetiawan and O. Gunnarsson, Phys. Rev. B **49**, 16 214 (1994).

[17] F. Aryasetiawan and O. Gunnarsson, Rep. Prog. Phys. **61**, 237 (1998).

[18] W.-D. Schöne and A. G. Eguiluz, Phys. Rev. Lett. **81**, 1662 (1998).

[19] B. Holm and U. von Barth, Phys. Rev. B **57**, 2108 (1998).

[20] F. Aryasetiawan, Phys. Rev. B **46**, 13 051 (1992).