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Electronic structure and electron-phonon coupling in stoichiometric and defective hydrides MPdH$_3$ (M=Ca, Sr, Eu, Yb)

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On the basis of electron transfer from the divalent element to the PdH$_3$ entities, the perovskite structure MPdH$_3$ (M=Sr, Eu, Yb) are expected to have similar electronic states at the Fermi energy as superconducting Pd-H$_x$ and Pd–noble-metal–H$_x$ and thus could be potential candidates for superconductivity. With this motivation, we have investigated the electronic structure and some aspects of the electron-phonon coupling in these hydrides using the *ab initio* augmented plane-wave method, and the results of the energy bands, the total and partial wave analysis of the density of states, and the electronic contribution, η_H to the electron-phonon coupling are presented. Similar studies for the hydrogen defective material CaPdH$_2$ are also included. We have found that all these compounds are metallic with essentially filled Pd-d bands and a small density of states at Fermi level as in PdH. Nevertheless, the calculated values of η_H, which govern the contribution of the hydrogen atoms to the electron-optical phonon coupling parameter λ, although sizeable, are lower than in PdH. This would indicate that these compounds, if superconducting, would have lower values of the superconducting transition temperatures T_c than in PdH. [S0163-1829(96)06146-2]

I. INTRODUCTION

To date, only a small number of metal hydrides have been found to be superconducting.[1] The most investigated system is PdH$_x$ (for $x \geqslant 0.8$) which has a maximum superconducting critical temperature T_c of 9 K with a remarkable inverse isotope effect since $T_c \approx 11$ K for PdD. The critical temperature can be further increased up to about 17 K in hydrogen charged Pd–noble-metal alloys such as Pd$_{0.55}$Cu$_{0.45}$H$_{0.7}$. For the Pd-H(D) system, neutron scattering,[2] superconducting tunneling,[3] temperature dependence of the resistivity,[4] as well as theoretical results[5] demonstrated that the electron-optical phonon coupling is primarily responsible for this high value of T_c. The substantial value of T_c arises due to the low-energy optic phonons and to the presence of a sizeable density of hydrogen s states at Fermi energy n_H (E_F) which insures the coupling to the hydrogen vibrations. The systematic calculation of the electron-optical phonon coupling constant λ_H in a series of transition-metal hydrides showed that n_H (E_F) is substantial essentially in metal hydrides with filled d bands.[6] These ideas have guided the synthesis of new hydrides with filled d bands which could possibly be superconducting. Palladium-based hydrides have thus been investigated. Palladium reacts with monovalent (alkali) and divalent (alkaline and rare earth) metal hydrides under hydrogen atmosphere to form complex hydrides. However, the search for superconducting hydrides has led to positive results only in a very limited number of compounds such as NaPd$_3$H$_2$ which can be viewed as a distorted sodium substituted palladium hydride, it is metallic and superconducting below 2 K.[7,8] Among the recently synthesized compounds, LiPdH$_x$ ($x \leqslant 1$) (Refs. 9–11) shows metallic behavior down to 4 K; Li$_2$PdH$_2$ and Na$_2$PdH$_2$ which are both characterized by linear PdH$_2$ complexes have a metallic conductivity,[12,13] while K$_2$PdH$_4$ is an insulator with square planar PdH$_4$ units.[14] Another example of hydrides containing palladium and divalent metals is Ca$_3$Pd$_2$H$_4$,[15,16] for which the intermetallic compound Ca$_3$Pd$_2$ exists.

CaPdH$_2$ along with SrPdH$_3$, EuPdH$_3$, and YbPdH$_3$, were recently synthesized by Bronger and co-workers.[17,18] The three compounds MPdH$_3$ (M=Sr, Eu, Yb) crystallize in a cubic perovskite structure, the Pd-H distances are however shorter than in PdH (see Table I). It is interesting to note that the complex quaternary hydride PdSr$_2$LiH$_5$ (Ref. 19) has been synthesized; it can be viewed as resulting from the stacking of two cubic perovskites units, the already investigated phase SrLiH$_3$ (Ref. 20) and the defective SrPdH$_2$ hydride. In our previous study of the electronic properties of PdSr$_2$LiH$_5$,[21,22] we have also analyzed the subunits SrLiH$_3$ (Ref. 23) and SrPdH$_3$ (with the lattice parameter of the quaternary hydride).

In the present work, we have investigated the electronic structure and the electron-optical phonon coupling in the series of hydrides MPdH$_3$ (M=Sr, Eu, Yb) and their evolution as a function of the internal pressure effect associated with the lattice contraction. In fact, the MPdH$_x$ (M=Sr, Eu, Yb) hydrides are slightly substoichiometric[18] (x=2.7, 2.9, and 2.7, respectively), but we assume these hydrides to be fully stoichiometric crystals. This is not the case for CaPdH$_2$ which is surprisingly hydrogen defective. Comparing the lattice constants of MPdH$_3$ to that of CaPdH$_2$, there is appar-

TABLE I. Lattice parameters and Pd-H distance (in Å) for various Pd-based hydrides.

	a	d(Pd-H)
SrPdH$_3$	3.839 (Ref. 18)	1.920
EuPdH$_3$	3.806 (Ref. 18)	1.903
YbPdH$_3$	3.710 (Ref. 18)	1.855
CaPdH$_2$	3.690 (Ref. 17)	1.841
PdH	4.095 (Ref. 31)	2.042

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ently no reason to consider that the missing hydrogen in this structure results in dramatic changes in the cell volume. For these rather new compounds, the phase diagram is frequently poorly determined or unknown. Consequently, it is reasonable to suppose that the fully stoichiometric compound $CaPdH_3$ could be prepared under adequate thermodynamic conditions. For this reason, we undertook also the study of the hydride $CaPdH_3$ along with the defective, experimentally observed, phase $CaPdH_2$. In the following sections we give a short summary of the technical aspects of the method and we discuss the results of the band structure, total density of states (DOS) and partial DOS of this series of hydrides. Finally, we discuss the calculated values of the electronic part of the electron-optical phonon coupling constant for these materials.

II. DETAILS OF THE CALCULATION

We have used the augmented plane-wave[24] (APW) method to calculate the energy bands of these hydrides with the experimental lattice parameters listed in Table I. The crystal potential was modelled in the muffin-tin approximation and the exchange term in the local-density approximation Slater X_α form which has proved to be adequate to study these types of materials.[21–23] We sampled 1/48 of the cubic Brillouin zone with 20 **k** points calculated *ab initio* with a convergence criterion on energy better than 1 mRy. The energy bands as well as the coefficients of the wave functions were fitted with a set of symmetrized plane waves. The uncertainty in this procedure is lower than 2 mRy. The total DOS as well the partial wave analysis of the DOS at each atomic site were calculated by means of the linear energy tetrahedron integration scheme.[25] The valence f electrons of Eu and Yb were obviously considered in the muffin-tin potential calculation but were removed from the APW matrix elements, since it is well known that highly correlated electrons are not correctly treated by one-electron methods. For the defective hydride $CaPdH_2$ the effect of disorder in the hydrogen sublattice was simulated by taking a weighted average of the structure factor over the 3H sites.

III. RESULTS AND DISCUSSION

A. Electronic structure

In Figs. 1(a), 2(a)–2(c), 3(a) we show the energy bands along some high-symmetry directions of the cubic Brillouin zone, the total DOS, and the partial wave analysis of the DOS inside each muffin-tin for the hydrides MPdH$_3$ (M=Sr, Eu, Yb). At the center of the cubic Brillouin zone Γ, we obtain for the three hydrides in increasing order of energy, a state of bonding H-s/Pd-s/M-s character followed by doubly degenerate bonding Pd-d_{e_g}/H-s states. The next triply degenerate level at Γ is formed essentially by the Pd-$d_{t_{2g}}$ nonbonding orbitals having lobes pointing away from the next-nearest neighbors of palladium. At higher energies, a doubly degenerate antibonding Pd-d_{e_g}/H-s state is found at the Brillouin-zone center. The energy difference between this antibonding state and its bonding counterpart at low energy increases from 0.598 to 0.660 Ry as the lattice parameter contracts by 3.36% from M=Sr to M=Yb.

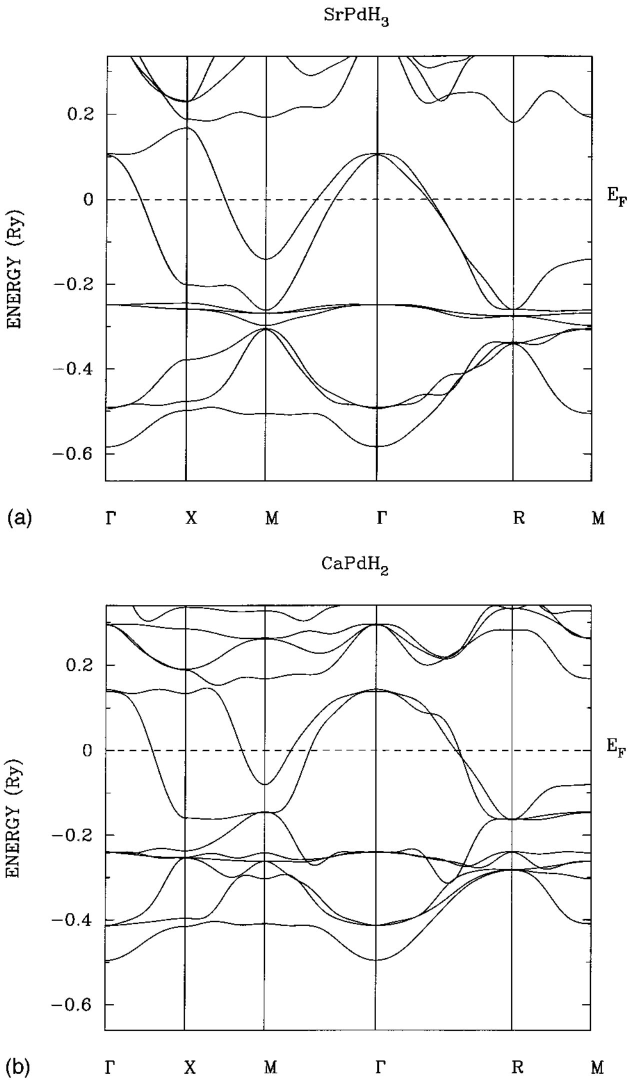

FIG. 1. Energy bands of (a) $SrPdH_3$ and (b) $CaPdH_2$.

The first structure in the DOS at low energy is composed of the first three metal-hydrogen bonding bands. Its width increases from 0.279 Ry (M=Sr) to 0.284 Ry (M=Eu) and 0.302 Ry (M=Yb) as the lattice parameter decreases. This is due to the increased overlap between the orbitals of neighboring atoms. The second structure in the DOS is a very narrow peak of high intensity due to the essentially nonbonding narrow Pd-$d_{t_{2g}}$ bands. The width of this structure increases also somewhat from 0.053 Ry (M=Sr) to 0.055 Ry (M=Eu) and 0.066 Ry (M=Yb) with decreasing lattice parameter. Finally, the last structure in the DOS is wide and of low intensity; it is due to the two antibonding metal-hydrogen bands.

Since the hydrides under study have 15 valence electrons, the first six bands up to the Pd-$d_{t_{2g}}$ narrow manifold are entirely filled, the remaining three electrons fill partially the overlapping antibonding metal-hydrogen bands. The hydrides are found to be metallic with a low DOS at E_F, respectively, 9.93, 10.03, and 9.13 states of both spins/Ry unit cell for M=Sr, Eu, Yb. The total DOS at E_F is dominated by the contribution of the Pd-d states, however, in this metal-hydrogen antibonding region, the H-s states are non-

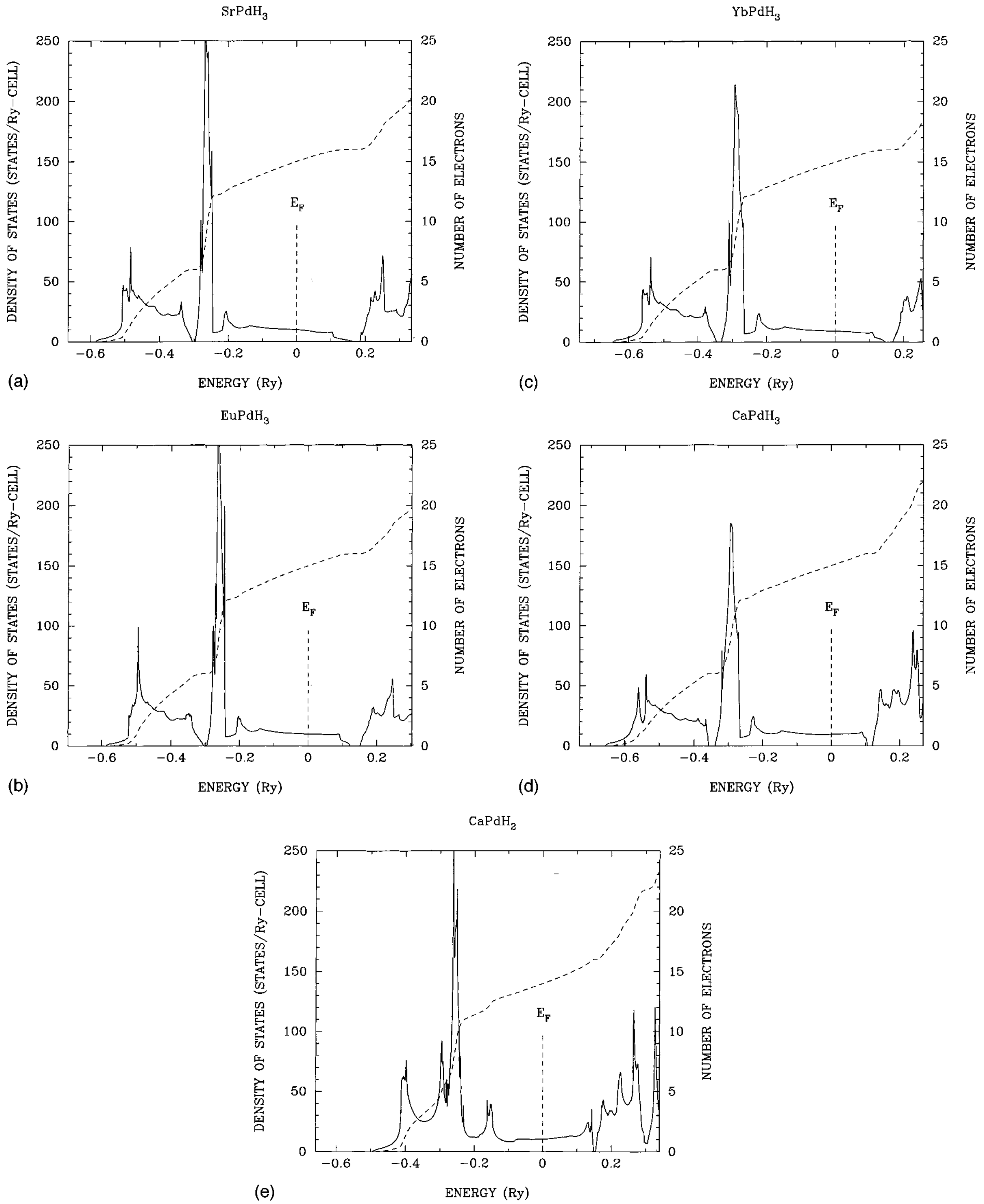

FIG. 2. Total density of states of (a) $SrPdH_3$, (b) $EuPdH_3$, (c) $YbPdH_3$, (d) $CaPdH_3$, and (e) $CaPdH_2$. The zero of the energy scale corresponds to the Fermi level.

negligible since they represent more than 10% of the Pd-*d* dominant contribution. A small contribution of the Sr-*d* states at E_F is also present in these compounds, which is of same order of magnitude as the H-*s* contribution. The value of the DOS at E_F is similar to that found for PdH, another hydride with filled Pd-*d* bands as shown in the DOS plot in Fig. 4.

The partial wave analysis shows very clearly the composition of the different bands. The first three bands are dominated by the Pd-*d*/H-*s* bonding interaction with a much smaller contribution of the Sr-*d*, Pd, and Sr *s* and *p* states. The next three narrow bands correspond to the nonbonding Pd-*d* states with a small Sr contribution. As just discussed, the two wide antibonding bands crossing the Fermi level result essentially from Pd-*d* states with non-negligible H-*s* and Sr-*d* contributions. At higher energies, from band 9 and up, the structure in the DOS is essentially due to the divalent metal-*d* states.

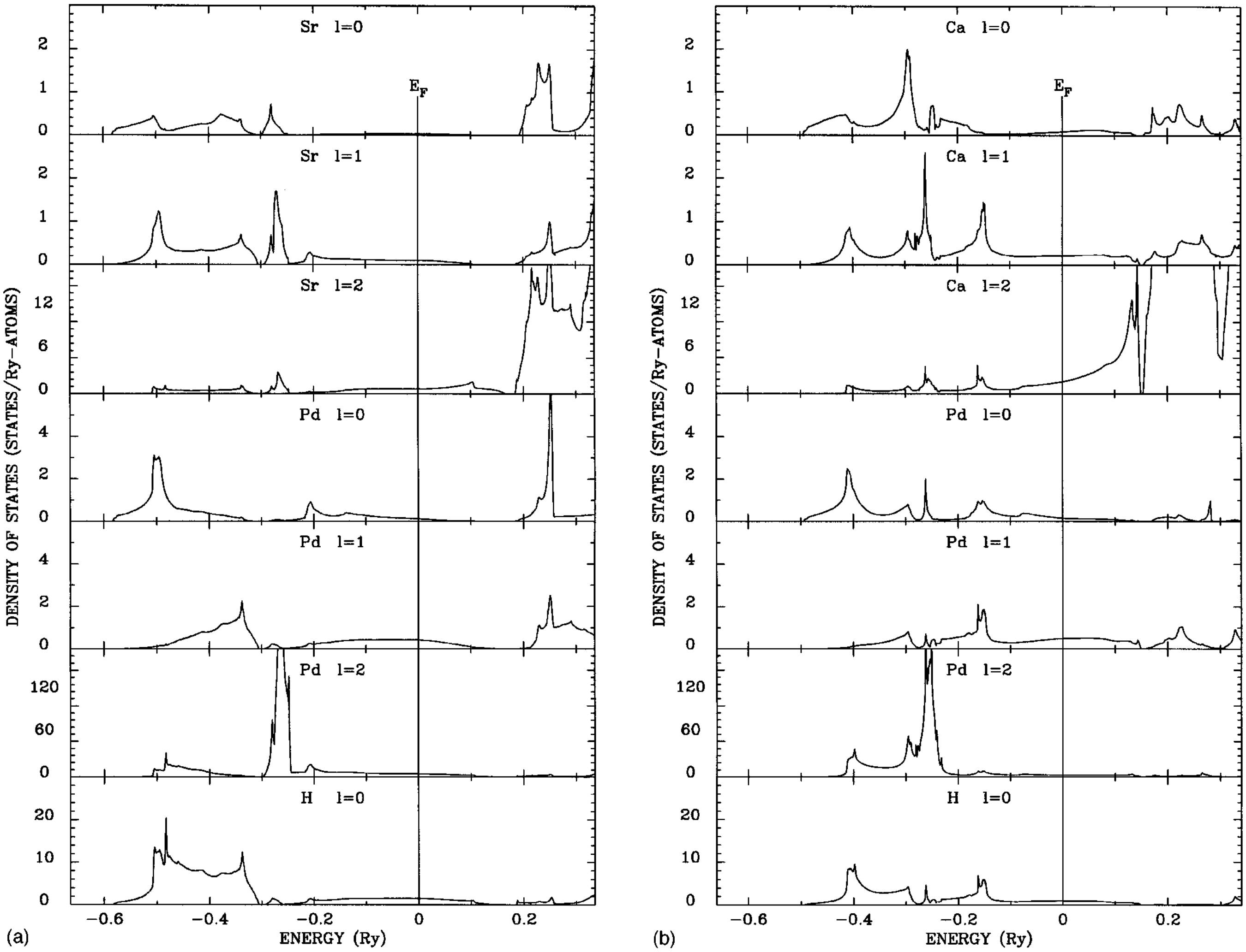

FIG. 3. Partial wave analysis of the density of states of (a) $SrPdH_3$ and (b) $CaPdH_2$ inside the muffin-tin spheres. Units are states/Ry atoms of the same type in the unit cell. The zero of the energy scale corresponds to the Fermi level.

In Figs. 1(b), 2(d), 2(e), and 3(b) we show the energy bands, total DOS and the partial wave analysis of the DOS of the cubic hydrides $CaPdH_3$ and $CaPdH_2$. In these figures, it can be clearly seen that the low-energy metal-hydrogen bonding bands of $CaPdH_2$ are much more narrow than in the trihydrides; their width is only 0.243 Ry and they are located at higher energies closer to the peak of the Pd-$d_{t_{2g}}$ states. This feature can be understood in terms of a weakening of the Pd-hydrogen interactions with decreasing hydrogen content and thus with a destabilization of the palladium hydrogen bonding bands. The partial wave analysis of the DOS reveals also that the Ca-d states participate in the bonding with hydrogen. They give rise to a structure in the DOS of $CaPdH_2$ around -0.16 Ry, above the narrow Pd-$d_{t_{2g}}$ peak. Such interaction between the divalent element-d and the H-s orbitals is not observed in this energy range in the series of hydrides $MPdH_3$ (M=Sr, Eu, Yb). This is due to the fact that the Ca-d states are the lowest in the divalent element series.

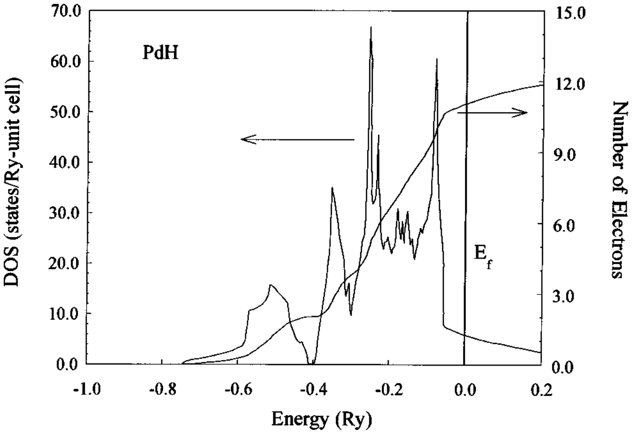

FIG. 4. Total density of states of PdH (Ref. 6).

In the defective hydride, as well as in the series of trihydrides, the low-energy metal-hydrogen bonding states as well as the narrow Pd-$d_{t_{2g}}$ bands are filled and the Fermi level crosses the two Pd-H antibonding bands hybridized with Ca-d states. The Fermi level of the defective hydride is however closer to the Pd-$d_{t_{2g}}$ peak of the DOS than in the trihydrides since $CaPdH_2$ has only 14 instead of 15 valence electrons. The total width of the antibonding bands is smaller

TABLE II. Density of states at Fermi energy $n(E_F)$ (in states of both spins/Ry unit cell), electronic specific-heat coefficient γ (in mJ K^{-2} mol^{-1}) and Pauli susceptibility χ_P (in mJ T^{-2} mol^{-1}) for the ternary hydrides under study and PdH_x.

	$n(E_F)$	γ	χ_P
$SrPdH_3$	9.934	1.721	0.0236
$EuPdH_3$	10.030	1.738	0.0238
$YbPdH_3$	9.131	1.582	0.0217
$CaPdH_3$	9.500	1.646	0.0226
$CaPdH_2$	10.440	1.809	0.0248
PdH_1 (calculated, Ref. 33)	6.602	1.144	0.0157
PdH_x (experimental)		1.53 ($x=0.89$) (Ref. 32)	0.016 ($x=0.71$) (Ref. 34)

in $CaPdH_2$ than in the $MPdH_3$ hydrides. This feature, which is correlated with the weak Pd-H interaction in the defective hydride, results in a slight increase in the value of the total DOS at E_F which is found to be 10.44 states of both spins/Ry unit cell in $CaPdH_2$. We find that the H-*s* contribution at E_F is slightly larger than in the trihydrides, due to an enhanced H-s/M-d interaction in this energy range. The Ca-*d* contribution at E_F in $CaPdH_2$ and $CaPdH_3$ is also larger than in the other divalent elements ($M=$Sr, Eu, Yb). This is associated with the lower position of the Ca-*d* states and can be clearly seen in the partial wave DOS curve corresponding to $1=2$ at the Ca site.

As mentioned previously, the stoichiometric hydride $CaPdH_3$ has not yet been synthetized. In the present electronic structure calculation we find that the DOS of $CaPdH_3$ is rather similar, for the width and position of the bonding bands as well as the Fermi energy position, to that of $YbPdH_3$ which has almost the same lattice parameter. The only small differences between these two trihydrides are found in the composition of the states at E_F and will result in subtle variations in the electron-optical phonon coupling discussed below.

Thus there is no obvious electronic factor which could prevent the formation of this trihydride. We hope that this point will be confirmed experimentally by using different thermodynamic conditions during synthesis. Let us recall in this connection that although stoichiometric PdH exists, hydrogen loading in PdH_x above $x\approx 0.7$ is rather difficult.

Besides the structural data, no experimental determination of other observables are yet available to date on the hydrides under study. From our calculated value of the density of states at the Fermi energy we can obtain in the noninteracting electron approximation, the unenhanced values of the electronic specific-heat coefficient γ and the Pauli susceptibility χ_P. The corresponding results are listed in Table II. These are of the same order of magnitude as the calculated and experimental values obtained for PdH_x which are also given for comparison. The bare calculated values of γ and χ_P are expected to be enhanced by the electron-phonon interaction and a variety of other factors.

The shape of the total DOS of the occupied states, plotted in Figs. 2(a)–2(e), could be compared to the results of photoemission experiments. We predict for the $MPdH_3$ compounds ($M=$Ca, Sr, Eu, Yb) that the Fermi energy E_F falls in a region of weak and slowly varying portion of the DOS. A large and narrow peak associated with the Pd-$d_{t_{2g}}$ bands should appear around 3.7 eV below E_F in the photoemission spectra as well as a low-energy structure of weaker intensity centered around 6.8 eV below E_F which results from the H-H and metal-hydrogen interactions. The x-ray emission spectroscopy can provide further information on the site and angular momentum dependence of the occupied states. Since the electronic transitions from the occupied conduction band to the core hole are governed by the dipole selection rule, our calculated Pd-*d* $(1=2)$ partial wave analysis of the DOS can be considered, for example, as a prediction of the shape of the Pd-$L_{II,III}$ spectrum. To sample the unoccupied states which we predict to be dominated by the divalent element-*d* partial wave contribution, it would be useful to obtain the divalent elements $L_{II,III}$ near edge absorption spectra. We hope that our calculations will stimulate further experimental work.

B. Electron-phonon coupling

The electronic states at the Fermi energy of the metals under study present some similarities with those of superconducting PdH. As in PdH, we find that the metal *d* bands are filled and we obtain a small but sizeable contribution of H-*s* states at E_F since the Fermi level cuts as in PdH the metal-hydrogen antibonding states.

The most direct experimental evidence of the applicability of the electron-optical phonon coupling mechanism in palladium hydrides (deuterides) stems from the superconducting tunneling experiments performed on the Pd-H(D) system.[3] From tunneling current-voltage characteristics the Eliashberg function function $\alpha^2(\omega)F(\omega)$ has been derived, where $F(\omega)$ is the phonon density of states and $\alpha^2(\omega)$ an averaged electron-phonon coupling constant. The maxima obtained in the Eliashberg function, which determines essentially the electron-phonon coupling constant λ, are well correlated with the position of the optic phonon peak in the phonon density of states derived from the neutron-scattering data.[2] This is a direct demonstration of the importance of the optic mode contribution to superconductivity in this material. These results have been confirmed by an analysis of the temperature dependence of the resistivity[4] as well as by theoretical evaluations.[5,6] The role of anharmonic phonon contributions and of larger zero-point motion of H compared to D has been invoked to interpret the inverse isotope effect observed between PdH and PdD in terms of a stiffening of the force constants.[26]

The analysis on the Pd-H(D) system revealed the importance of two factors: the low average value of the frequency

TABLE III. Electronic part of the electron-optical phonon coupling constant η_α (in eV Å^{-2})

	η_M	$\eta_{\rm Pd}$	$\eta_{\rm H}$
$SrPdH_3$	0.06	0.23	0.43
$EuPdH_3$	0.06	0.23	0.39
$YbPdH_3$	0.05	0.23	0.43
$CaPdH_3$	0.07	0.20	0.35
$CaPdH_2$	0.12	0.28	0.51
PdH		0.87	0.64 (Ref. 6)

of the optic modes [$\hbar\omega_{\rm opt}\approx 56$ meV in PdH (Ref. 2)] and the presence of H-s states at E_F which enhance the electronic contribution of the electron-optical phonon coupling constant $\lambda_{\rm H}$. These states are a sizeable fraction of the total DOS at E_F only for hydrides with filled d bands such as PdH and the five hydrides investigated here.

We have thus calculated the electronic contribution to λ, denoted hereafter η, by means of the Gaspari-Gyorffy model developed in the framework of McMillan's approximation,[27,28]

$$\lambda=\sum_\alpha \lambda_\alpha=\sum_\alpha \frac{\eta_\alpha}{M_\alpha\langle\omega^2\rangle_\alpha}, \tag{1}$$

$$\eta_\alpha=\frac{E_F}{N_\uparrow(E_F)\pi^2}\sum_l 2(l+1)\sin^2(\delta_{l+1}^\alpha-\delta_l^\alpha)\times\frac{n_l^\alpha(E_F)n_{l+1}^\alpha(E_F)}{n_l^{\alpha\rm ss}(E_F)n_{l+1}^{\alpha\rm ss}(E_F)}. \tag{2}$$

In Eq. (2), $N_\uparrow$ is the total DOS (for one spin) and n_l^α is the partial DOS of angular momentum l projected at the atomic-site α. The label ss stands for single site scatterers, and δ_l^α are the phase shifts for the atom α. All these quantities are evaluated at the Fermi energy, E_F.

In Table III we summarize the results of η calculated for the five hydrides. The rather weak values η_M for the divalent metal yield, after being weighted by the atomic mass, a negligible contribution to λ. Slightly larger values of the electronic contribution $\eta_{\rm Pd}$ are found for the Pd atom in these compounds, however, these values as in the case of PdH are much smaller than those obtained for superconducting transition metals[29,30] and should lead to small values of $\lambda_{\rm Pd}$.

In contrast, we find that the hydrogen contributions, $\eta_{\rm H}$ are sizeable for the five compounds, although lower than in superconducting PdH ($\eta_{\rm H}=0.64$ eV Å^{-2}).[6] The difference between the values of $\eta_{\rm H}$ found between the three hydrides of the series $MPdH_3$ can be explained as follows. The contribution at E_F of the H-s density of states decreases consistently with the lattice contraction from M=Sr to Eu and Yb. This leads to a corresponding decrease in the value of the angular momentum sum appearing in Eq. (2). However, the value of the Fermi energy E_F which appears in the prefactor of Eq. (2) varies in the opposite way since it increases from Sr to Eu and Yb relative to the bottom of the conduction band. This feature is due to the energy lowering of the metal-hydrogen bonding bands accompanying the decrease of the Pd-H distances. The interplay of the antagonist variations of E_F and of the angular momentum sum lead to equal values of $\eta_{\rm H}$ for $SrPdH_3$ and $YbPdH_3$. The value of $\eta_{\rm H}$ obtained for $EuPdH_3$ is slightly smaller than for the other compounds of the series. This difference is enhanced by the larger value of the total DOS at E_F, which appears in the denominator of the prefactor in Eq. (2). The hypothetical trihydride $CaPdH_3$ is found to have the smallest value of $\eta_{\rm H}$. This is due to a smaller H-s-contribution at E_F associated with a larger Ca-d hybridization. The value of $\eta_{\rm H}$ obtained for $CaPdH_2$ is even larger than that of $SrPdH_3$ and $YbPdH_3$. This is due to the increased H-s-contribution at E_F since in the defective compound, the energy difference between bonding and antibonding metal H-s states decreases. However, this value of $\eta_{\rm H}$ remains smaller than that calculated for PdH cited previously.

The trihydrides under study are thus quite similar to PdH; however the calculated values of $\eta_{\rm H}$ are about 35% smaller than in PdH. In both cases, a palladium atom remains octahedrally coordinated; however, the coordination of H atoms by Pd atoms is not the same. While in PdH, the hydrogens are also octahedrally coordinated by the Pd atoms, in $MPdH_3$ compounds, they have only twofold colinear coordination. This substantially weakens the interaction of the H atoms with Pd atoms in $MPdH_3$ and hence reduces the values of $\eta_{\rm H}$.

Although the experimental lattice parameters of substoichiometric hydrides have been used in the present calculations, we expect very small changes in the predicted values of $\eta_{\rm H}$ because the Fermi energy falls in a very flat and slowly varying portion of the density of states. The electronic states will thus be very midly affected by a small modification of the lattice parameter. The optic phonon frequencies, not considered here, are expected to be more sensitive than $\eta_{\rm H}$ to changes in the Pd-H bond lengths.

We have no experimental data on the average frequencies of the optic modes $\langle\omega^2\rangle_{\rm H}$; however a hardening of the optic phonons could be expected from the reduced Pd-H distances in these trihydrides. Such hardening would further decrease the value of $\lambda_{\rm H}$. However, since in BCS theory the prefactor in the expression of the superconducting transition temperature T_c is proportional to the average phonon frequencies, we cannot further speculate on the possible values of T_c for these hydrides. Nevertheless, we believe that these trihydrides are interesting candidates for low-T_c superconductivity and we hope that the present investigation will stimulate further experimental work in this direction.

IV. CONCLUSIONS

The electronic properties of the cubic perovskite hydrides $MPdH_3$ (M=Sr, Eu, Yb), hypothetical $CaPdH_3$ and the defective hydride $CaPdH_2$ present great similarities since the occupied electronic states result mostly from the Pd-d/H-s and H-s/H-s interactions which are very similar in these isostructural systems. The divalent element s, p, and d orbitals participate also in the bonding but give a much weaker contribution and a large fraction of the two electrons of the divalent element are essentially transferred to the Pd and H states located at lower energies. In the series $MPdH_3$, the observed differences stem essentially from the chemical pressure effect associated with the lattice contraction. This effect is responsible for the larger width and the energy lowering of the three metal-hydrogen bonding bands, for the slight broadening of the Pd-$d_{t_{2g}}$ peak and for some subtle differences in the character of the states at Fermi energy.

The calcium compound $CaPdH_2$ presents larger differences with the other hydrides $MPdH_3$ due to the weakening of the Pd-H interactions in this substoichiometric system and to a larger contribution of Ca-*d* states to the bonding, a feature expected in view of the relative position of the atomic unoccupied divalent element *d* states.

In all cases, the Pd-*d* bands are essentially filled and the Fermi energy crosses the antibonding metal-hydrogen bands as in superconducting PdH. The densities of states at E_F of these metallic perovskites are low, as in PdH and noble metals.

The electronic contribution η_H to the electron-optical phonon coupling constant λ_H have sizeable values due to the presence of H-*s* states at E_F. However the values obtained for η_H remain somewhat smaller than those calculated within the same model for superconducting PdH. We could not give estimates of λ_H due to the lack of experimental data on the phonon frequencies, however these metallic perovskite hydrides could be considered as possible candidates for low-T_c superconductivity. It is our hope that the present work will stimulate further experimental investigations concerning the nature of superconductivity or lack of it in these compounds.

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