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Electron Landé g factor in GaAs–(Ga,Al)As quantum wells under applied magnetic fields: Effects of Dresselhaus spin splitting

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The effects of the Dresselhaus spin splitting on the Landé g factor associated with conduction electrons in GaAs–(Ga,Al)As quantum wells are studied by using the nonparabolic Ogg–McCombe effective Hamiltonian. The g factor and cyclotron effective mass are calculated as functions of applied magnetic fields (along both the growth and in-plane directions) and GaAs well widths of the heterostructure. Present calculations indicate that in GaAs–(Ga,Al)As heterostructures, the inclusion of the Dresselhaus term leads to very small corrections in the effective Landé factor. Taking into account the effects of nonparabolic and anisotropic terms in the Hamiltonian is fundamental in obtaining quantitative agreement with experimental measurements. Moreover, the present results suggest that previous theoretical work on the Dresselhaus spin-splitting effects on the effective Landé factor should be viewed with caution if nonparabolic and anisotropic effects are not taken into account. © 2008 American Institute of Physics. [DOI: 10.1063/1.2956698]

I. INTRODUCTION

Some properties of conduction-electron states in low-dimensional systems depend very much on the understanding of the interaction of the electron spins, not only with the solid-state environment but also with external probes like applied magnetic fields. Due to the possible applications in a variety of semiconductor devices based on spin-electronic transport,1 this has been the subject of considerable interest in the last decade or so. A special interest has been focused on the study of the Landé g factor of GaAs–(Ga,Al)As semiconductor heterostructures, which is related to the spin splitting of carrier bands, and may be very different from the corresponding free-electron values. The spin-splitting of electron levels influences the spin dynamics and spin resonance and may give rise to a wide range of technological applications based on the manipulation of the g factor and cyclotron mass of carriers by means of changes in the heterostructure geometry, application of external magnetic fields, hydrostatic pressure, etc. Experimental measurements on the Landé g factor and cyclotron effective mass may provide valuable information on the electronic band structure and on the importance of effects such as nonparabolicity and anisotropy. Here we should mention that in GaAs–(Ga,Al)As heterostructures, it is a known fact that the Dresselhaus contribution to the conduction-band electronic structure is small, although its comparative importance with other nonparabolic/anisotropic effects over the electronic states in semiconductor heterostructures does not seem to have attracted much attention.

The present study is essentially concerned with the combined effects of the Dresselhaus spin-splitting and nonparabolic/anisotropic terms on the effective Landé factor and cyclotron effective mass associated with conduction electrons in GaAs–(Ga,Al)As quantum wells (QWs) under an externally applied magnetic field. Section II describes the present theoretical framework and the procedures to solve the Schrödinger equation corresponding to the Ogg–McCombe effective Hamiltonian under magnetic fields applied both parallel and perpendicular to the QW growth axis and gives expressions to evaluate the electron Landé factor and cyclotron effective mass in such systems. Section III is concerned with the present theoretical results and discussion. Conclusions are given in Section IV.

II. THEORETICAL FRAMEWORK

In the present work, we use the Ogg–McCombe effective Hamiltonian2–5 for the conduction-band electrons in a GaAs–Ga1−xAlxAs QW under a magnetic field \( \mathbf{B} \) in the \( z \)-direction, i.e.,

\[
\hat{H} = \hat{H}_0 + \hat{W},
\]

with

\[ \hat{H}_0 = \frac{p^2}{2m_e} + \frac{1}{2} m_e \omega_c^2 z^2 - \frac{1}{2} g \mu_B B z, \]

\[ \hat{W} = \vec{B} \cdot \hat{\tau}, \]

where \( m_e \) is the electron effective mass, \( \omega_c \) is the cyclotron frequency, \( g \) is the Landé factor, \( \mu_B \) is the Bohr magneton, and \( \vec{B} \) is the magnetic field.
\[ \hat{H}_0 = \frac{\hbar^2}{2m} \mathbf{K} \cdot \mathbf{\hat{r}} + V(\mathbf{r}) + \frac{1}{2} g \mu_B B \hat{\sigma}_z + \alpha_1 \hat{K}^2 \mathbf{\hat{r}} + \frac{\alpha_2}{l_B^2} \hat{I}_y + \alpha_3 \hat{K}^2 \mathbf{\hat{r}} + \alpha_4 B_2 \hat{K}^2 \mathbf{\hat{r}}_z + \alpha_5 B_1 (\hat{\sigma} \cdot \mathbf{K}) \mathbf{\hat{r}}_z + \alpha_6 B \hat{\sigma}_z \mathbf{\hat{r}}_z, \]

where the orthogonal axes \( x, y, \) and \( z \) were taken along the principal crystallographic directions.\(^3\) \( \mathbf{K} \) is the \( 2 \times 2 \) matrix unit, \( l_B = \sqrt{\hbar/eB} \) is the Landau length, \( \mu_B \) is the Bohr magneton, \( \mathbf{K} = \mathbf{\hat{r}} + (e/\hbar c) \mathbf{A} \) [we chose the gauge \( \mathbf{A} = (-yB, 0, 0) \) for the magnetic vector potential], \( \mathbf{\hat{r}} = -i \nabla, \) \( \hat{\sigma} \) is a vector which components are the Pauli matrices, \( \mathbf{\hat{r}}_z = \mathbf{\hat{K}} \mathbf{\hat{r}}_z \mathbf{\hat{K}} \) and its corresponding cyclic permutations, whereas \( m, g, \) and \( V \) are the growth-direction position-dependent effective mass, Landé factors, and confining potential, respectively, for conduction electrons in the QW heterostructure.\(^4\) The coefficients \( a_i \) \((i = 1, 2, \ldots, 6)\) are constants which are, in principle, different on both the well and barrier materials. However, forced by the absence of experimental measurements on the behavior of the \( a_i \) coefficients as functions of the aluminum concentration in Ga\(_{1-x}\)Al\(_x\)As and related materials, we have taken the \( a_i \) values corresponding to bulk GaAs and obtained by a fitting with magnetoreflectance and spectrometric measurements.\(^5\) The operator \( \mathbf{\hat{W}} \) is the cubic Dresselhaus spin-orbit term\(^6\) associated with the Ga\(_{1-x}\)Al\(_x\)As lack of inversion symmetry, and the Dresselhaus constant \( \Gamma \) exhibits a step-like dependence on the position along the growth direction, i.e., \( \Gamma = \Gamma(x) \), which leads to the so-called interface Dresselhaus spin-orbit coupling.\(^7,8\) The magnitude of the \( \Gamma \) discontinuity at the interfaces of the QW may be found via the dependence of \( \Gamma \) on the aluminum concentration \( x \) in Ga\(_{1-x}\)Al\(_x\)As. The values of \( \Gamma \) experimentally measured for GaAs oscillate in the range between 20 and 35 eV \( \Lambda^3 \)\(^9\). Following de Dios-Leyva et al.\(^4\) and Cardona et al.\(^10\), here we have used \( \Gamma = \Gamma(0) \approx 20 \) eV \( \Lambda^3 \) for GaAs. Using \( \Gamma(1) = 18.53 \) eV \( \Lambda^3 \) for AlAs, as reported by Winkler,\(^11\) one may linearly interpolate and propose \( \Gamma(x) = \Gamma(1) - 1.47x \) (eV \( \Lambda^3 \)) for the Dresselhaus constant as a function of the aluminum concentration. We note that in a GaAs–Ga\(_{0.95}\)Al\(_{0.05}\)As QW, for example, the \( \Gamma \) discontinuity is about 2.6% of the \( \Gamma \) value corresponding to bulk GaAs, and one may expect that the inclusion of the position dependence on \( \Gamma \) along the growth direction will result in a small correction to the effective \( g \) factor in the heterostructure. We have, therefore, assumed \( \Gamma \) as constant and equal to the GaAs value throughout the heterostructure.

We study two possible configurations of the applied magnetic field: magnetic fields applied parallel to the growth direction (\( B_\parallel \) configuration) of the QW, and in-plane applied magnetic fields, \( i.e., \) magnetic fields applied parallel to the heterostructure layers (\( B_\perp \) configuration). Both configurations require different procedures to solve the Schrödinger equation associated with the above Ogg–McCombe Hamiltonian.

### A. \( B_\parallel \) configuration

Here we take the GaAs–Ga\(_{1-x}\)Al\(_x\)As QW as grown along the \( z \)-direction. Therefore, the electron effective mass, Landé factor, and confining potential are taken as \( z \)-dependent functions and the \( z \)-direction applied magnetic field is parallel to the growth axis. As \( \mathbf{\hat{W}} \) does not depend explicitly on \( x \) in this case, the eigenfunctions of Eq. (1) may be chosen as

\[ \Psi(r) = \begin{pmatrix} \Phi^+(y,z) \\ \Phi^-(y,z) \end{pmatrix} \exp(\pm i\kappa_z z), \]

and by introducing \( y' = y - \frac{\hbar}{m} \dot{\kappa}_z \) and the annihilation \( \dot{a} = \begin{pmatrix} 1/\sqrt{2} [y'/l_B + ik_z/l_B] \end{pmatrix} \) and creation \( \dot{a} \) operators, the Ogg–McCombe Hamiltonian may be transformed into\(^4\)

\[ \hat{H} = \hat{H}_0 + \mathbf{\hat{W}}. \]

where

\[ \hat{H}_0 = \begin{pmatrix} \hat{\chi}_0^+ & 0 \\ 0 & \hat{\chi}_0^- \end{pmatrix}, \]

\[ \hat{\chi}_0^+ = \hat{\chi}_0^- + \hat{\chi}_0^+ \theta \mathbf{\hat{r}}_z \mathbf{\hat{r}}_z + \hat{\chi}_0^+ \beta \mathbf{\hat{r}}_z \mathbf{\hat{r}}_z, \]

\[ \hat{\chi}_0^+ = \frac{\hbar^2}{2m(z)} (a_4 + a_5 + a_6)B + 4a_1 + a_3 \dot{N}, \]

\[ \hat{\chi}_0^+ = \frac{2a_2}{l_B^2} + \frac{2}{l_B^2} \left[ \frac{\hbar^2}{2m(z)} + a_4 \dot{N} \right], \]

and \( \dot{N} = \dot{\theta} + 1/2 \). The operator \( \mathbf{\hat{W}} \) in Eq. (5) is given by

\[ \mathbf{\hat{W}} = \begin{pmatrix} \mathbf{\hat{W}}_1 & \mathbf{\hat{W}}_2 \\ \mathbf{\hat{W}}_2 & \mathbf{\hat{W}}_1 \end{pmatrix}, \]

where

\[ \mathbf{\hat{W}}_1 = \begin{pmatrix} -a_3 & \Gamma/l_B^2(a_4 + a_5) \\ \Gamma/l_B^2(a_4 + a_5) & -a_3 \end{pmatrix}, \]

\[ \mathbf{\hat{W}}_2 = \begin{pmatrix} -2a_3B\dot{\kappa}_z + \Gamma a_4 \dot{\kappa}_z^2 & \Gamma/2l_B^2 \dot{\kappa}_z^2 - \Gamma/2l_B^2 (\dot{\kappa}_z^2 - \dot{\kappa}_z^2) \\ \Gamma/2l_B^2 (\dot{\kappa}_z^2 - \dot{\kappa}_z^2) & -2a_3 \dot{\kappa}_z^2 + \Gamma a_4 \dot{\kappa}_z^2 \end{pmatrix}, \]

As previously pointed out by Golubev et al.\(^3\) and de Dios-Leyva et al.\(^4\) the characteristic problem for \( \hat{H}_0 \) may be solved analytically, and the operator \( \mathbf{\hat{W}} \) only contributes with a minor correction to the energy levels. Therefore, one may
solve the Schrödinger equation in the $B_\parallel$ configuration by
using perturbation theory up to second order, which is suffi-
cient for reaching a good agreement between theoretical re-
sults and experimental measurements (see below).

B. $B_\perp$ configuration

One may now consider the GaAs–Ga$_{1-x}$Al$_x$As QW as
grown along the $y$-direction. The $z$-direction applied mag-
netic field is then perpendicular to the growth direction, and
therefore, as $\hat{H}$ [cf. Eq. (1)] does not explicitly depend on $x$
and $z$, $k_x$ and $k_z$ are good quantum numbers. The eigenfunc-
tions of $\hat{H}$ may then be chosen as
\[
\Psi(\mathbf{\vec{r}}) = \begin{pmatrix} \Phi^+(y) \\ \Phi^-(y) \end{pmatrix} \exp[i(k_x x + k_z z)] / \sqrt{L_x L_z},
\]
where $L_x$ and $L_z$ are the heterostructure lengths along the $x$
and $z$ direction, respectively. It is important to note that the
combined effects of the heterostructure confining potential
and applied in-plane magnetic field lead to a dependence of
the eigenvalues of $\hat{H}$ on the cyclotron orbit-center position
$y_0 = k_x l_B^2$. At low temperatures only the lowest energy levels
are occupied and $k_z = 0$ is a good approximation. In this case,
the operator $\hat{H}_0$ becomes diagonal and the diagonal compo-
nents of $\hat{W}$ vanish. The Schrödinger equation for the two-
component wave function then leads to
\[
\begin{pmatrix} \hat{H}_0^+ \\ \hat{W}_{21} \end{pmatrix} \Psi^+(y) = \begin{pmatrix} \Phi^+(y) \\ \Phi^-(y) \end{pmatrix},
\]
where $\hat{H}_0^+$ and $\hat{W}_{21}$ are the diagonal components of Eq. (2),
describing the spin-up and spin-down electron states, respec-
tively, in the absence of the Dresselhaus spin-orbit term, and
the operators $\hat{W}_{12}$ and $\hat{W}_{21}$ are given by
\[
\hat{W}_{12} = \Gamma \begin{pmatrix} \hat{k}_x (k_x - \frac{y}{l_B^2}) \hat{k}_y + i (k_x - \frac{y}{l_B^2}) \hat{k}_y (k_y - \frac{y}{l_B^2}) \end{pmatrix},
\]
\[
\hat{W}_{21} = \Gamma \begin{pmatrix} \hat{k}_x (k_x - \frac{y}{l_B^2}) \hat{k}_y - i (k_x - \frac{y}{l_B^2}) \hat{k}_y (k_y - \frac{y}{l_B^2}) \end{pmatrix},
\]
respectively, or, by using the creation and annihilation oper-
ators,
\[
\hat{W}_{12} = \frac{\Gamma}{\sqrt{2l_B^2}} (\hat{a}^\dagger \hat{a}^3 - \hat{a}^3 \hat{a}^\dagger)
\]
and
\[
\hat{W}_{21} = \frac{\Gamma}{\sqrt{2l_B^2}} (\hat{a} \hat{a}^3 - \hat{a}^3 \hat{a}).
\]
Equation (16) may be readily solved by expanding the two-
component wave function Eq. (15) in a series of the harmonic-
ocillator wave functions $|n, y_0\rangle$, i.e.,
\[
\begin{pmatrix} \Phi^+(y) \\ \Phi^-(y) \end{pmatrix} = \sum_n \begin{pmatrix} C_n^+ \\ C_n^- \end{pmatrix} |n, y_0\rangle,
\]
where $\langle n, y_0 | y, y_0 \rangle = \sqrt{1/(2\pi n! \sqrt{\pi l_B})} e^{-(y-y_0)^2/(4l_B^2)} H_n[(y-
y_0)/l_B]$ are the harmonic-oscillator wave functions written
in the coordinate representation, and $H_n$ are the Hermite
polynomials.

C. The effective Landé factor and cyclotron effective mass

The inclusion of the Dresselhaus contribution in the
Ogg–McCombe Hamiltonian requires taking into account the
off-diagonal terms in $\hat{H}$, which mix the different spin states
in the semiconductor heterostructure. However, due to the
expected slight effects of the Dresselhaus contribution on the
electron-energy spectrum in GaAs–Ga$_{1-x}$Al$_x$As semicon-
ductor heterostructures,

\begin{align}
E_n^{(\pm)} &= \frac{E_n^{(\pm)}(\alpha) - E_{n+1}^{(\pm)}(\alpha)}{\mu_B B},
\end{align}

where $\alpha$ means “$|$” or “$\perp$”, according to the magnetic-field
direction. In addition, for a given direction of the applied
magnetic field and for a given subset of spin-up-like or spin-
down-like electron states, the $m_c$ cyclotron effective mass
associated with the $n$th and $(n+1)$-th Landau magnetic sub-
bands may be defined by
\[
E_{n+1}^{(\pm)} - E_n^{(\pm)} = \hbar eB / m_c^{(\pm)}.
\]
Of course, the effective Landé factor as well as the cyclotron
effective mass will, in principle, depend on the applied mag-
netic field strength, and in the case of the $B_\perp$ configuration,
they also depend on the orbit-center position.

III. RESULTS AND DISCUSSION

In contrast to previous work, we have considered here
the role played by the cubic Dresselhaus spin-orbit coupling
on the cyclotron-effective mass and Landé factor in
GaAs–Ga$_{1-x}$Al$_x$As semiconductor QWs under magnetic
fields applied parallel or perpendicular to the layers. Figure 1
shows the increase of the cyclotron effective mass
for $n=0$ in the above equation as either the in-plane or
growth-direction applied magnetic field increases in comparison
with the bulk GaAs value [cf. Fig. 1(a)], and its decrease as the
QW width increases [cf. Fig. 1(b)]. It is apparent that the
effect of the Dresselhaus term (here we have chosen for
the conduction-electron cyclotron effective mass is negligible, as calculated results with or without in-
clusion of the Dresselhaus effect are essentially indistin-
guishable in the scale of Fig. 1. The higher value of the
cyclotron electron effective mass for the growth-direction...
applied magnetic field, as compared with the result for the in-plane applied field, is related to the strong barrier-confining effects in the in-plane magnetic-field orientation. For a given value of the in-plane magnetic field and for such a small-width ($L=50$ Å) QW, due to presence of the Ga$_{0.65}$Al$_{0.35}$As barrier, the electron wave function is essentially inside the QW (the barrier-confinement potential is much stronger than the effect of the in-plane magnetic field), leading to a smaller cyclotron electron effective mass. Present results for the growth-direction applied magnetic field are in good agreement with experimental results by Singleton et al. and Michels et al.

The dependence of the perpendicular Landé $g_{\perp}$ factor ($n=0$) with the orbit-center position is presented in Fig. 2. As expected, it increases with the strength of the in-plane applied magnetic field, and with both the strength ($\Gamma$ value) of the Dresselhaus term and proximity of the orbit-center to the Ga$_{0.65}$Al$_{0.35}$As barrier. This is due to differences in the electron energies between the spin-up-like and spin-down-like electron states which increase not only by the action of the applied magnetic field, but by the repulsion of the electron wave function by the barriers of the QW structure (which the electron must tunnel in this field orientation). Notice, however, that at low temperatures (zero orbit-center position), the perpendicular Landé $g_{\perp}$ factor practically does not depend on the strength of the Dresselhaus term. It is possible to show that the effects of the Dresselhaus contribution to the effective Landé factor are proportional to the ratio $\Gamma'/(\hbar\omega_B)^2$. Particularly in GaAs and related materials, the above-mentioned ratio is much less than 1 in the range of magnetic fields up to 20 T. Actually, the contribution of the Dresselhaus spin-orbit coupling does not vanish as the orbit-center position tends toward zero, as a straightforward calculation indicates that the matrix elements $\langle y_0, n | W_{12} | m, y_0 \rangle$ and $\langle y_0, n | W_{21} | m, y_0 \rangle$ do not depend on $y_0$. The more remarkable dependence of the effective $g_{\perp}$ factor as a function of the orbit-center position for $\Gamma \neq 0$ than for $\Gamma=0$ may be understood in terms of the mixing effects of the different spin states due to the presence of the off-diagonal elements in the Hamiltonian when the Dresselhaus spin-orbit coupling is taken into account.

As mentioned before, one of the factors that modifies the effective Landé factor is the electronic spin interactions with the solid-state environment (QW confining potential) and external probes like an applied magnetic field. In Fig. 3 one observes an increase of the perpendicular Landé $g_{\perp}$ factor with the strength of the applied magnetic field as well as with increasing quantum confinement, i.e., as the GaAs QW width diminishes.

The parallel and perpendicular conduction-electron Landé $g$ factors are presented in Fig. 4 (calculations were performed for a vanishingly small value of the applied magnetic field), in comparison with experimental results, for $\Gamma=0$ (no Dresselhaus term) and $\Gamma=20$ eV Å$^3$. Figure 4 also shows insets presenting the results corresponding to the contribution of the cubic spin-orbit (Dresselhaus) term to the effective Landé factor. Notice that for both magnetic field configurations, the theoretical results essentially do not depend on the value of the strength $\Gamma$ of the Dresselhaus term, except for minor changes in the parallel case for small QW widths.

**FIG. 1.** Cyclotron effective mass, in units of the free-electron mass $m_0$, as a function of (a) the applied magnetic field for $L=50$ Å and (b) the QW width for $B=4$ T in GaAs–Ga$_{0.65}$Al$_{0.35}$As QWs both in the $B_1$ and $B_2$ configurations. Theoretical results are shown for the spin-up-like states. Open symbols in (b) are the experimental measurements reported by Singleton et al. (Ref. 12) and Michels et al. (Ref. 13). For the case of in-plane magnetic fields ($B_2$), the orbit-center position was taken at $y_0=0$. Solid (dashed) lines correspond to $\Gamma=20$ eV Å$^3$ ($\Gamma=0$). Calculations for bulk GaAs are also displayed.

**FIG. 2.** Orbit-center-position dependence of the effective $g_{\perp}$ factor in a 20 Å-width GaAs–Ga$_{0.65}$Al$_{0.35}$As QW for two different values of the in-plane magnetic field ($y_0=0$ at the center of the well). Solid and dashed lines correspond to a Dresselhaus constant $\Gamma=20$ eV Å$^3$ and $\Gamma=0$, respectively.

**FIG. 3.** Landé $g_{\perp}$ factor as a function of the in-plane magnetic field in GaAs–Ga$_{0.65}$Al$_{0.35}$As QWs for various values of the well width. Theoretical results were performed for the orbit-center position at the center of the QWs ($y_0=0$). Solid and dashed lines correspond to $\Gamma=20$ eV Å$^3$ and $\Gamma=0$, respectively. Calculations for bulk GaAs are also displayed.
widths. The agreement with experimental results is excellent in both configurations. Furthermore, it is clear from Fig. 4 that one should take into account the effects of the anisotropic terms in the Ogg–McCombe Hamiltonian in order to find good agreement with the available experimental results.

We display in Fig. 5 the anisotropy of the effective Landé factor as a function of the QW width for GaAs–Ga0.65Al0.35As QWs at $B=4$ T. Solid and dashed lines correspond to $\Gamma=20$ eV Å$^3$ and $\Gamma=0$, respectively. Solid circles correspond to the experimental measurements of Malinowski and Harley (Ref. 16).

**IV. CONCLUSIONS**

Summing up, present calculated results in GaAs–Ga0.65Al0.35As QWs demonstrate that the inclusion of effects of the Dresselhaus term on the calculation of the conduction-electron effective $g$ factor represents very small corrections with respect to the effects of nonparabolic and anisotropic terms. Of course, the above statement is only valid for GaAs and related materials, for which the Dresselhaus constant reaches moderate values. For other materials with large Dresselhaus spin-orbit coupling, such as InSb or GaSb, the Dresselhaus parameter $\Gamma$ is more than 10 times larger than for GaAs and, therefore, one may expect that the effects of the Dresselhaus spin-orbit coupling may not be small. The present study presents a clear indication that any realistic calculation of the effective Landé factor for semiconductor heterostructures must include the nonparabolic/anisotropic terms in the model Hamiltonian in order to obtain a quantitative understanding of experimental results. We should point out that nonparabolicity and anisotropic effects in the conduction band may also be taken into account through a calculation in which conduction, valence, and higher band effects are considered within the same theoretical framework in a multiband (Kane, 8 × 8, 14 × 14, multiband schemes) calculation. As a final conclusion, we stress that one should be cautious with results and conclusions of previous parabolic conduction-band studies which do not appropriately take into account nonparabolic and anisotropic effects in the calculation/analysis of the Landé $g$ factor in low-dimensional semiconductor systems.

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4V. G. Golubev, V. I. Ivanov-Omskii, I. G. Minervin, A. V. Osatin, and D. G. Polyakov, Sov. Phys. JETP 61, 1214 (1985) [we have used their values for \((a_1, a_2, a_3) = (-2.9, -2.6, -1.2) \times 10^6 \text{ meV Å}^2\text{ and } (a_4, a_5, a_6) = (-9.7, -0.8, 4.9) \text{ meV Å}^2/T \text{ in the present theoretical calculations.}]


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