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All-electron local-density and generalized-gradient calculations of the structural properties of semiconductors

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The lattice constant, bulk modulus, and single-particle eigenvalues of Si, Ge, and GaAs are evaluated by using the local-density approximation (LDA) and the generalized-gradient approximation (GGA) for the exchange-correlation energy. We consider two different generalized-gradient functionals, the exchange correlation recently proposed by Perdew and Wang and the Becke exchange combined with a previous version of the Perdew-Wang correlation. We perform an all-electron calculation with the linear-augmented-plane-wave method to test the capability of these generalized-gradient-exchange-correlation functionals to describe structural properties of semiconductor systems. Our results differ from previous calculations of the same quantities within the pseudopotential scheme although the qualitative trends are the same. The LDA yields lattice constants that are smaller by less than 0.6% than the experimental values. Both GGA's overcorrect, giving lattice constants that are larger than the experimental ones by about 2% for the earlier GGA and by about 1.5% for the later GGA. The LDA predicts bulk moduli that are within 3% of the experimental value whereas the GGA's underestimate the bulk moduli by 14–22%. The underestimate of the LDA band gaps is not improved by either of the GGA's.

I. INTRODUCTION

Within density functional theory, the ground state energy of an interacting system of electrons in an external potential can be written as a functional of the ground state electronic density.[1,2] The theory is, in principle, exact but the energy functional contains an unknown quantity, the exchange-correlation energy $E_{\rm xc}[\rho]$, which has to be approximated. The local-density approximation (LDA) is a widely used approximation of the exchange-correlation functional,

$$E_{\rm xc}^{\rm LDA}[\rho] = \int d\mathbf{r}\, \rho\, \epsilon^{\rm LDA}(\rho). \tag{1}$$

$E_{\rm xc}^{\rm LDA}$ represents the exact functional for a homogeneous electron gas and has been shown to give also a qualitatively good description of the ground state properties of a variety of highly inhomogeneous systems. However, LDA does not always provide sufficiently accurate results. For example, it almost always overestimates the binding energy and often underestimates the bond length of molecules and solids especially in weakly bound cases.[3] LDA fails also to predict the ground state structure of iron.[4] In the attempt to improve upon LDA, a dependence of the exchange-correlation energy on the derivatives of the electronic density can be introduced. This approximation is known as the generalized-gradient approximation (GGA). The generalized-gradient approximation exchange-correlation energy restricted to first-order derivatives is

$$E_{\rm xc}^{\rm GGA}[\rho] = \int d\mathbf{r} \rho\, \epsilon^{\rm GGA}(\rho, |\nabla\rho|). \tag{2}$$

Up to the present time, several generalized-gradient approximation functionals have been proposed by different authors both for the exchange and the correlation energy.[5–12] The Becke exchange[6] combined with the Perdew correlation functional[7] (BP), the Perdew-Wang exchange-correlation[7,8] (PW86), and the more recent version of the same functional[9,10] (PW91) are among the most commonly used functionals and have been tested by using different computational schemes. These approximate functionals seem to give a good description of several finite systems: they improve the values of the total energy of atoms,[13] the cohesive energy, equilibrium distance, and vibration frequency of weakly bound molecules (IIA-IIB dimers),[14] the cohesive energy of most first-row and second-row molecules[15] and of atomic clusters.[16] They also give a better estimate of the cohesive energy of simple metals,[13] third row elements,[17] and hydrogen bonded systems.[18] For iron, the correct ferromagnetic bcc ground state is predicted[17] as well as the correct high pressure phase transition.[19] While there is general agreement about the improvement yielded by the GGA upon the LDA in the description of the structural

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properties of 3d transition metals,[17,20–23] contradictory results have been found for 4d and 5d metals.[22–24] For these systems, different theoretical schemes have been used to solve the Kohn-Sham equations and the approximations introduced in these methods make it difficult to establish the accuracy of the functionals. The same problem is encountered in the literature regarding semiconductor systems. Si, Ge, and GaAs have been studied within the pseudopotential approach in combination with different generalized-gradient approximation functionals. The pseudopotentials have been constructed either in the density functional LDA scheme and screened within the generalized-gradient approximation[22,25] or generated including gradient corrections[14] and applied to bulk systems with and without nonlinear core corrections.[26–28]

Here, we report tests of the PW91 GGA functional[9] and a functional consisting of the Becke exchange[6] combined with the earlier PW86 correlation functional (BP) (Ref. 7) for the semiconductors, Si, Ge, and GaAs and compare the results to those obtained from LDA.[10] The calculations were performed using the general potential linear-augmented-plane-wave (LAPW) method.[29,30] This method differs from pseudopotential approaches in that it makes no frozen core or related approximations and permits treatment of the Ga and Ge 3d states on the same footing as the valence states. Additionally, the method uses a very flexible basis while imposing no shape approximations on either charge density or potential.

In Sec. II, we give a brief outline of the method used and describe the characteristics of our calculations. In Sec. III, we present our results and a comparison with the values obtained by other authors.

II. METHOD

The general potential LAPW method has been reviewed in detail elsewhere.[30] Accordingly, only aspects specific to the present calculation are presented here. Both the core and valence states are treated self-consistently, the core states relativistically and the valence states in a scalar relativistic approximation. Spin orbit for the valence states is, however, included for the calculation of the band structures of GaAs and Ge, using a second variational approach.[30] Highly converged basis sets constructed with $R_{\rm MT}G_{\rm max}$ equal to nine are used ($R_{\rm MT}$ is the LAPW sphere radius, demoted $R_{\rm MT}$ for historical reasons–a muffin-tin potential is not implied–and $G_{\rm max}$ is the interstitial plane-wave cutoff). For instance, for Si in LDA, reducing $R_{\rm MT}G_{\rm max}$ to 8.5 results in a change in the energy of only few tens of μRy. Additional local orbital basis functions are used to include the Ga and Ge 3d states in the same energy window as the valence states as well as to remove any errors due to the energy linearization. The zone samplings during iteration to self-consistency are performed using 10 special k points[31] in the irreducible wedge of the zone. Increasing the sampling to 60 special k points changes the total energy of Si and GaAs by a few tenths of a mRy and that of Ge by approximately 1 mRy. The larger change in the total energy of Ge with respect to Si and GaAs is expected because both LDA and GGA predict Ge to be a semimetal instead of a semiconductor, at both the experimental and the theoretical equilibrium lattice constants, at least with the inclusion of spin-orbit coupling and for the particular parametrization of the LDA used.[10]

Tests are also performed to determine the sensitivity of the results to the LAPW sphere radii used in the calculation. This is important for GGA calculations because continuity of the second derivatives of the wave functions and, therefore, the charge density is not enforced in the LAPW method, and this then can lead to discontinuities in the GGA potential, which depends on these second derivatives. We find that the GGA lattice parameters and bulk moduli which we present here are insensitive to the choice of the radii. However, changes of a few tens of mRy are found in the value of the total energy of GaAs when the LAPW sphere radius is changed by 2.5%, while for LDA the change is only a few tenths of a mRy. Hence, we present cohesive energy for the LDA functional only.

III. RESULTS AND CONCLUSIONS

In Table I, we report our results for the equilibrium lattice constant and the bulk modulus of Si, Ge, and GaAs. We also list the results obtained by Juan and Kaxiras[28] using the LDA and the PW91 exchange-correlation functional and the pseudopotential method. The equilibrium lattice parameter for these systems was calculated by Ortiz[26] within the pseudopotential scheme and with the use of the LDA and the BP exchange correlation. Calculations of the lattice constant and bulk modulus of Si were also performed by Dal Corso *et al.*[27] using the same functionals and computational scheme as Ortiz. We compare only with these authors because they include the generalized-gradient functional in the construction of the pseudopotentials. Ortiz's results are closer to our all-electron calculations than Juan and Kaxiras's results for the respective exchange-correlation functionals. The relative difference between the LDA and the BP GGA lattice parameters found by Ortiz is very close to the difference we evaluate. Since the use of nonlinear core corrections brings Ortiz's BP GaAs lattice parameter close to ours, we could expect a better agreement between our results and Ortiz's results for all the systems both in the LDA and the GGA if nonlinear core corrections were included in all of Ortiz's calculations. For Si, Dal Corso *et al.* obtained a_0 = 10.20 a.u. and B_0 = 0.96 Mbar, within the LDA, in excellent agreement with our results. The pseudopotentials generated using the PW86 functional are known to have a pathological shape and to be, therefore, less transferable with respect to the smoother pseudopotentials obtained by using the BP functional.[14] The difference between the PW86 and BP functional is the exchange part of the functional. Juan and Kaxiras use the PW91 exchange correlation and we can, therefore, expect that the pseudopotentials generated including this approximate exchange-correlation functional will have similar or worse oscillations[34] and irregular behavior than the PW86 functional and will be less transferable than the BP pseudopotentials. Although Ortiz's results are closer to our all-electron calculations, the pseudopo-

TABLE I. LAPW calculations of the lattice constant and bulk modulus of Si, Ge, and GaAs by using the Perdew-Wang exchange-correlation functional (PW91) (Ref. 9) and the Becke exchange in combination with a previous version of the Perdew-Wang correlation functional (BP) (Ref. 7). We also list the results obtained by Juan and Kaxiras with the LDA and PW91 (Ref. 28) and by Ortiz with the LDA and BP (Ref. 26). For GaAs with BP, Ortiz obtains a_0 =10.80 a.u. and $-E_{\text{cohesive}}$ = 6.13 eV by including nonlinear core corrections. The numbers in parentheses are the percentage errors. The experimental values are as quoted in Ref. 28.

Crystal	Property	Present work			Juan and Kaxiras		Ortiz		Experiment
		LDA	PW91	BP	LDA	PW91	LDA	BP	
Si	a_0 (a.u.)	10.22(-0.4)	10.39(1.3)	10.46(1.9)	10.17(-0.9)	10.56(2.9)	10.15(-1.1)	10.38(1.2)	10.26
	B_0 (Mbar)	0.96(-3)	0.83(-16)	0.80(-19)	0.97(-2)	0.85(-14)			0.99
	$-E_{\text{cohesive}}$ (eV)	5.28(14)			5.38(16)	4.64(0.2)	5.35(16)	4.41(-4.8)	4.63
Ge	a_0 (a.u.)	10.63(-0.6)	10.86(1.6)	10.88(1.8)	10.53(-1.5)	11.19(4.7)	10.52(-1.6)	10.80(1)	10.69
	B_0 (Mbar)	0.78(1.3)	0.61(-21)	0.60(-22)	0.75(-2.6)	0.58(-25)			0.77
	$-E_{\text{cohesive}}$ (eV)	4.54(18)			4.53(18)	3.71(-3.6)	4.65(21)	3.68(-4.4)	3.85
GaAs	a_0 (a.u.)	10.62(-0.6)	10.84(1.5)	10.88(1.9)	10.42(-2.4)	11.19(4.8)	10.41(-2.5)	10.70(0.2)	10.68
	B_0 (Mbar)	0.74(-2.6)	0.65(-14)	0.60(-21)	0.77(1.3)	0.55(-28)			0.76
	$-E_{\text{cohesive}}$ (eV)	7.99(23)			8.58(32)	6.43(-1.4)	8.16(25)	6.45(-1.1)	6.52

TABLE II. Eigenvalues of the Kohn and Sham equations at Γ, X, and L for Si. All the eigenvalues are in eV and their zero is taken to be the top of the valence band ($\Gamma_{25'}$). The eigenvalues are evaluated at the experimental lattice parameter a_{exp} = 10.26 a.u. The experimental eigenvalues are as quoted in Ref. 33.

Si	Γ_1	Γ_{15}	X_1	X_4	X_1	$L_{2'}$	L_1	$L_{3'}$	L_1
LDA	-11.97	2.53	-7.83	-2.86	0.61	-9.63	-7.00	-1.20	1.42
PW91	-12.10	2.47	-7.91	-2.90	0.47	-9.73	-7.09	-1.21	1.38
BP	-12.08	2.53	-7.90	-2.87	0.59	-9.73	-7.05	-1.20	1.42
Expt.	-12.5±0.6	3.4		-2.9	1.13	-9.3±0.4	-6.8±0.2	-1.2±0.2	2.04±0.06

TABLE III. Eigenvalues of the Kohn and Sham equations at Γ, X, and L for Ge without spin-orbit interaction. All the eigenvalues are in eV and their zero is taken to be the top of the valence band ($\Gamma_{25'}$). The eigenvalues are evaluated at the experimental lattice parameter a_{exp} = 10.69 a.u. The experimental eigenvalues are as quoted in Ref. 26.

Ge	Γ_1	$\Gamma_{2'}$	X_1	X_4	X_1	$L_{2'}$	L_1	$L_{3'}$	L_1
LDA	-12.82	-0.19	-8.95	-3.08	0.66	-10.74	-7.65	-1.40	0.05
PW91	-12.85	-0.06	-8.94	-3.14	0.56	-10.74	-7.68	-1.43	0.05
BP	-12.83	-0.10	-8.94	-3.10	0.68	-10.74	-7.65	-1.42	0.09
Expt.	-12.9±0.2	0.89	-9.3±0.2	-3.5±0.2	1.3±0.5	-10.6±0.5	-7.7±0.2	-1.4±0.3	0.84

TABLE IV. Eigenvalues of the Kohn and Sham equations at Γ, X , and L for GaAs without spin-orbit interaction. All the eigenvalues are in eV and their zero is taken to be the top of the valence band ($\Gamma_{25'}$). The eigenvalues are evaluated at the experimental lattice parameter a_{exp} = 10.68 a.u. The experimental eigenvalues are as quoted in Ref. 33.

GaAs	Γ_1	Γ_1	X_1	X_3	X_5	X_1	L_2	L_1	L_3	L_1
LDA	-12.80	0.29	-10.29	-6.89	-2.69	1.35	-11.03	-6.70	-1.15	0.85
PW91	-12.80	0.40	-10.24	-6.91	-2.75	1.22	-11.00	-6.75	-1.17	0.84
BP	-12.79	0.39	-10.26	-6.90	-2.72	1.36	-11.01	-6.72	-1.16	0.88
Expt.	-13.1	1.63	-10.75	-6.70	-2.80	2.18	-11.24	-6.70	-1.30	1.85

TABLE V. Eigenvalues of the Kohn and Sham equations at Γ, X, and L for Ge with the inclusion of spin-orbit interaction. All the eigenvalues are in eV and their zero is taken to be the top of the valence band (Γ_8^+). The eigenvalues are evaluated at the experimental lattice parameter a_{exp} = 10.69 a.u. The experimental eigenvalues are as quoted in Ref. 32.

Ge	Γ_6^+	Γ_7^+	Γ_7^-	X_5	X_5	X_5	L_6^-	L_6^+	L_6^-	$L_{4,5}^-$	L_6^+
LDA	-12.93	-0.30	-0.29	-9.05	-3.18	0.56	-10.84	-7.75	-1.60	-1.41	-0.06
PW91	-12.94	-0.28	-0.16	-9.03	-3.23	0.46	-10.83	-7.78	-1.62	-1.44	-0.05
BP	-12.92	-0.28	-0.20	-9.03	-3.20	0.59	-10.83	-7.74	-1.60	-1.43	-0.004
Expt.	-12.9±0.2	-0.3	0.9	-9.3±0.2	-3.5±0.2	1.3±0.2	-10.6±0.5	-7.7±0.2	-1.4±0.3	-1.4±0.3	4.2±0.1
	-12.6				-3.15±0.2						4.3±0.2

TABLE VI. Eigenvalues of the Kohn and Sham equations at Γ, X, and L for GaAs with the inclusion of spin-orbit interaction. All the eigenvalues are in eV and their zero is taken to be the top of the valence band (Γ_8). The eigenvalues are evaluated at the experimental lattice parameter $a_{\mathrm{exp}} = 10.68$ a.u. The experimental eigenvalues are as quoted in Refs. 33 and 35.

GaAs	Γ_6	Γ_7	Γ_6	X_6	X_7	X_6	X_7	X_6	L_6	L_6	L_6	L_5	L_6
LDA	-12.91	-0.34	0.17	-10.41	-7.00	-2.85	-2.76	1.23	-11.14	-6.82	-1.36	-1.16	0.73
PW91	-12.91	-0.33	0.29	-10.35	-7.02	-2.90	-2.82	1.11	-11.11	-6.86	-1.38	-1.18	0.73
BP	-12.90	-0.33	0.27	-10.37	-7.01	-2.87	-2.79	1.25	-11.12	-6.83	-1.37	-1.17	0.77
Expt.	-13.21	-0.33	1.52	-10.86	-6.81	-2.93	-2.86	2.07	-11.35	-6.81	-1.46	-1.36	1.74

tential approach provides a description of the structural properties of these semiconductor systems that is not in complete quantitative agreement with our calculations while the qualitative trends are predicted to be the same. Both GGA's overcorrect the local-density approximation equilibrium lattice parameters. The lattice parameter is too small in the LDA by 0.4–0.6 % but it is too large by 1.3–1.6 % for PW91 and by 1.8–1.9 % for BP. While the LDA gives bulk moduli that are within 3% of the experimental values, the GGA's underestimate the bulk moduli by 14–22 %.

In Tables II, III, and IV, we present the Kohn-Sham eigenvalues and the experimental excitation energies at Γ, X, and L for Si, Ge, and GaAs without spin-orbit splitting. In Tables V and VI, we include the spin-orbit splitting for Ge and GaAs. The eigenvalues are evaluated at the experimental lattice constant in order to isolate the effects due to the different functionals. Although the excitation spectrum is not given by the single-particle eigenvalues of the true density functional,[35] this comparison is nevertheless frequently made. As is well known, LDA greatly underestimates the band gap of Si and GaAs and for Ge it gives a band overlap at Γ. The GGA and LDA eigenvalues are not much different if they are evaluated at the same (experimental) lattice constant. The band gap tends to open up under lattice compression. Hence, evaluation of the eigenvalues at the theoretical value of the lattice constant makes the direct LDA band gap somewhat larger for all three systems and the direct GGA band gaps somewhat smaller. For GaAs, both GGA's give a small band overlap at Γ when spin-orbit interaction is included. Comparison with the pseudopotential results of Ortiz show that the eigenvalues for Si agree to better than 0.1 eV but the largest discrepancies for Ge and GaAs are 0.19 eV and 0.26 eV, respectively. This is because Ortiz constructed the pseudopotentials for Ge and Ga with the relatively shallow $3d$ states in the core. The Ge and Ga $3d$ states are at -25 eV and -15 eV, respectively and the overlap with the valence states is not negligible. The error introduced by treating the $3d$ states as core states can be partly cured if nonlinear core corrections are included. For GaAs, with the BP functional, Ortiz does use nonlinear core corrections and the resulting eigenvalues are in somewhat better agreement with ours. The error can be completely removed only if the d states are not frozen as core states. The importance of relaxing the Ga d states and including relativistic corrections is discussed in Ref. 36. The omission of relativity and core relaxation results in an accidental better agreement with the experimental band gap. A recent pseudopotential calculation[37] using a hardness conserving pseudopotential (which include nonlinear core corrections) (Ref. 38) yields LDA eigenvalues that agree with ours to better than 0.02 eV for Si, 0.1 eV for Ge, and 0.15 for GaAs. The fact that the discrepancies are largest for GaAs, which has the shallowest d band, points to the omission of the d states from the valence as being the largest remaining error.

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