



An alternative way of linearizing the augmented plane-wave method

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Received 1 September 1999; accepted 16 December 1999 by P. Dederichs

Abstract

A new basis set for a full potential treatment of crystal electronic structures is presented and compared to that of the well-known linearized augmented plane-wave (LAPW) method. The basis set consists of *energy-independent* augmented plane-wave functions combined with local orbitals. Each basis function is continuous over the whole unit cell but it may have a discontinuous slope at the muffin-tin boundaries, i.e. at the surfaces of atomic centered, non-overlapping spheres. This alternative way to linearize the augmented plane-wave method is shown to reproduce the accurate results of the LAPW method, but using a smaller basis set size. The reduction in number of basis functions is most significant for open structures. © 2000 Elsevier Science Ltd. All rights reserved.

Keywords: A. Surfaces and interfaces; D. Electronic band structure

1. Introduction

Since Slater first proposed the method in 1937, augmented plane-wave (APW) and its descendents [1–3] have been among the most popular methods for solving the electronic structure using the density-functional theory [4,5]. In part, this popularity arose from the fact that the APW method in its modern general potential linearized forms combines a conceptual simplicity with high accuracy for a general system. The method uses a smaller basis set than soft pseudo-potential plane-wave basis approaches, but still substantially larger than local function methods like the linear-muffin-tin-orbital (LMTO) method or Gaussian-orbital techniques.

During the years, there have been several important developments of the original APW method, e.g. the full potential implementation [6,7] as well as inclusion of atomic forces [8,9]. But without doubt the single most important step was the linearization of the secular problem as proposed by Andersen [10]. In the present paper we present an alternative way of linearizing the APW method that, unlike earlier approaches, does not demand substantially larger basis set size than that of the original APW method in

order for results to converge. When converged, the method yields numerically identical results to the conventional linearized APW (LAPW) method.

Sections 1.1 and 1.2 provide short backgrounds to the APW and LAPW methods, while in Sections 2 and 3 we present and demonstrate our linearization of the APW method.

1.1. The original augmented plane-wave method

All APW descendent methods divide space into atomic centered muffin-tin (MT) spheres surrounded by an interstitial region. The APW basis functions consist of plane-waves in the interstitial region, that are augmented into radial solutions of the Schrödinger equation inside the MT spheres. These radial functions u_l are better for describing the behavior of the Bloch eigenfunctions close to atomic sites. For a system with one atom per unit cell this gives:

$$\phi_{\mathbf{G}}^{\text{APW}}(\mathbf{r}, \mathbf{k}) = \begin{cases} e^{i\mathbf{k}_{\mathbf{G}} \cdot \mathbf{r}} & \mathbf{r} \in \text{I} \\ \sum_L d_L^{\mathbf{k}_{\mathbf{G}}} u_l(r, E) Y_L(\hat{\mathbf{r}}) & \mathbf{r} \in \text{MT}, \end{cases} \quad (1)$$

where \mathbf{G} is a reciprocal lattice vector, \mathbf{k} is the crystal momentum and $\mathbf{k}_{\mathbf{G}} = \mathbf{k} + \mathbf{G}$. L is the condensed angular momentum index $\{l, m\}$ and $Y_L(\hat{\mathbf{r}})$ the spherical harmonics.

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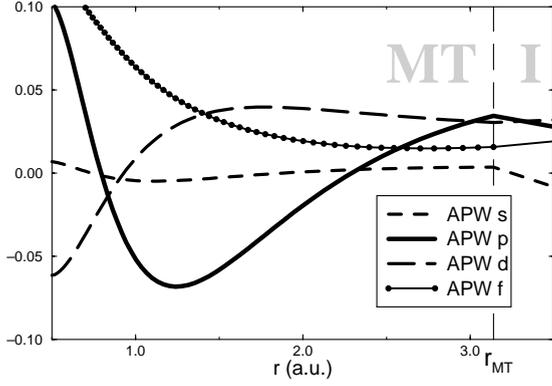


Fig. 1. Radial part u_l of the l -composition of an APW basis function for Ce. $\mathbf{k} = 2\pi/a$ (0.101, 0.208, 0.107), $\mathbf{G} = 2\pi/a$ (1, 1, 1). The radial solutions are evaluated at $\mathcal{E}_1 = 0.3$ Ry for the s-orbital and $\mathcal{E}_1 = 0.5$ Ry for all other orbitals.

In practical calculations the sum over L is finite. The coefficients $a_L^{\mathbf{k}_G}$ are found by expanding each plane-wave into Bessel functions $j_l(\mathbf{k}_G r)$ at the MT spheres, $r = r_{\text{MT}}$, requiring the basis functions to be continuous at the sphere boundaries. This yields

$$a_L^{\mathbf{k}_G} = 4\pi i^l Y_L^*(\hat{\mathbf{k}}_G) \frac{j_l(\mathbf{k}_G r_{\text{MT}})}{u_l(r_{\text{MT}}, E)}. \quad (2)$$

While the plane-waves are energy independent, the radial solutions u_l depend on the energy at which the radial Schrödinger equation is evaluated. An eigenfunction $\Psi_i(\mathbf{r}) = \sum_{\mathbf{G}} C_{i\mathbf{G}} \phi_{\mathbf{G}}(\mathbf{r}, \mathbf{k})$ can only be efficiently described by orbital solutions u_l evaluated at the eigenenergy \mathcal{E}_i of Ψ_i . A new set of APW basis functions must therefore be evaluated for each new energy treated. As the matrix elements representing operators depend on the choice of basis set the secular equation will be non-linear in energy.

$$\det[T_{\mathbf{G}\mathbf{G}'}(E) + V_{\mathbf{G}\mathbf{G}'}(E) - E\mathcal{O}_{\mathbf{G}\mathbf{G}'}(E)] = 0. \quad (3)$$

$T_{\mathbf{G}\mathbf{G}'}$ represents the kinetic energy operator; $V_{\mathbf{G}\mathbf{G}'}$ is the potential energy and $\mathcal{O}_{\mathbf{G}\mathbf{G}'}$ the overlap matrix. The procedure of evaluating the determinant for a number of different energies, in order to find the energy eigenvalues, makes the APW method very time consuming. Another problem is the decoupling of the basis set for energies yielding $u_l = 0$ at the MT-sphere boundary, but this is of less importance.

1.2. The linearized augmented plane-wave method

Parallel developments by Andersen [10] and Koelling and Arbman [11] resulted in the energy-independent LAPW basis functions,

$$\phi_{\mathbf{G}}^{\text{LAPW}}(\mathbf{r}, \mathbf{k}) = \begin{cases} e^{i\mathbf{k}_G \cdot \mathbf{r}} & \mathbf{r} \in \text{I} \\ \sum_L R_L^{\text{LAPW}}(r) Y_L(\hat{\mathbf{r}}) & \mathbf{r} \in \text{MT} \end{cases} \quad (4)$$

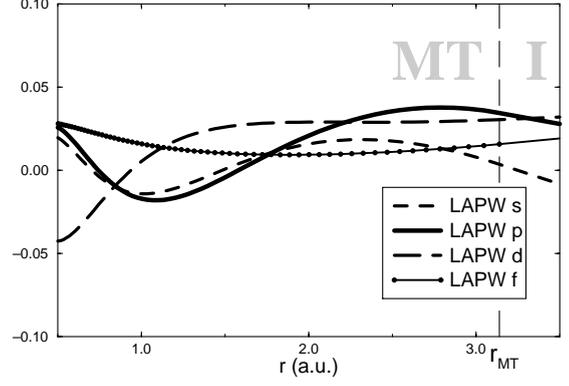


Fig. 2. Radial part R_L^{LAPW} of the l -composition of an LAPW basis function for Ce, evaluated at the same \mathbf{k} -point, \mathbf{G} -vector and energies as in Fig. 1.

where $R_L^{\text{LAPW}}(r) = a_L^{\mathbf{k}_G} u_l(r, \mathcal{E}_1) + b_L^{\mathbf{k}_G} \dot{u}_l(r, \mathcal{E}_1)$. $\dot{u}_l \equiv \partial u_l / \partial E$ are the energy derivatives of the radial functions. The two coefficients $a_L^{\mathbf{k}_G}$ and $b_L^{\mathbf{k}_G}$ are determined by forcing each basis function to be continuously differentiable, i.e. continuous with the continuous first derivative, at the surfaces of the MT spheres, see for example Ref. [3]. $u_l(r, \mathcal{E}_1)$ and $\dot{u}_l(r, \mathcal{E}_1)$ are evaluated for a linearization energy \mathcal{E}_1 , and $\phi_{\mathbf{G}}^{\text{LAPW}}$ provides sufficient basis for eigenfunctions in an energy range around this linearization energy. Thereby, the secular equation Eq. (3) becomes linear in energy, and all eigenenergies can be found through one diagonalization of the secular matrix. The cost of the energy-independent LAPW basis set is an increased number of basis functions compared to the APW method. Thus, the relatively large secular matrix of APW will be increased using the LAPW basis set.

2. An alternative way of linearizing: APW + lo

Is it possible to combine the advantages of the APW and LAPW methods, i.e. to find an energy-independent basis that does not demand a noticeable higher plane-wave cut-off than the original APW basis functions?

An energy-independent APW basis set alone does not provide enough flexibility to find solutions in a region around the fixed energy parameter. The variational freedom can be improved by using a complementary basis set consisting of local orbitals [12] for physically important l -quantum numbers, i.e. for $l \leq 3$. The local orbitals put no extra condition on the APW basis set, and the number of plane-waves in the interstitial is therefore unaffected.

Local orbitals were first introduced in the LAPW method by Singh [12] to treat semi-core states. They are local in the sense that they are completely confined within the MT

spheres,

$$\phi_L^{\text{lo}}(\mathbf{r}, \mathbf{k}) = \begin{cases} 0 & \mathbf{r} \in \text{I} \\ R_L^{\text{lo}}(r)Y_L(\hat{\mathbf{r}}) & \mathbf{r} \in \text{MT}. \end{cases} \quad (5)$$

In this work $R_L^{\text{lo}}(r) = a_L^{\text{lo}}u_l(r, \mathcal{E}_1) + b_L^{\text{lo}}\dot{u}_l(r, \mathcal{E}_1)$, using the same linearization energy \mathcal{E}_1 for all basis functions for simplicity. Changing the linearization energy slightly for the local orbitals should not effect the calculations. Further, the linearization energy can easily be chosen so that the decoupling of basis functions when $u_l(r_{\text{MT}}, \mathcal{E}_1)$ or $\dot{u}_l(r_{\text{MT}}, \mathcal{E}_1)$ equals zero is avoided. a_L^{lo} is set to 1 while b_L^{lo} is determined using $\phi_L^{\text{lo}} = 0$ at the MT boundary.

The new basis functions will hereafter be referred to as APW + lo. Once the scheme of local orbitals is implemented into an LAPW code the changes for turning it into APW + lo are straightforward. All developments within LAPW, such as the full potential implementation, work equally well for APW + lo.

2.1. The new basis in the MT region

The APW + lo basis functions, will differ in some important aspects from the LAPW basis functions inside the MT region.

Comparing the l -decompositions of an APW and an LAPW basis function in the MT region, Figs. 1 and 2, respectively, it is seen that the linear combinations $R_L^{\text{LAPW}}(r)$ of Eq. (4) differ considerably from the original solutions $u_l(r, \mathcal{E}_1)$ used in APW. Thereby, none of the energies in the interval around \mathcal{E}_1 , including \mathcal{E}_1 itself, is treated as exact by the LAPW basis set, as the single energy examined by one APW basis set. The APW + lo basis set, on the other hand, includes both $u_l(r, \mathcal{E}_1)$ in its original APW form for efficient description of eigenfunctions at energies close to \mathcal{E}_1 , and a (less restricted) linear combination of $u_l(r, \mathcal{E}_1)$ and $\dot{u}_l(r, \mathcal{E}_1)$ to improve the description of states away from \mathcal{E}_1 . The deformation of $R_L^{\text{LAPW}}(r)$ compared to $u_l(r, \mathcal{E}_1)$ in Fig. 2 is not dependent on the *magnitude* of the radius of MT, but on how well $u_l(r, \mathcal{E}_1)$ alone matches the Bessel function in value and derivative for a certain r_{MT} . For the rare case of perfect matching $b_L^{\text{kg}} = 0$ and $u_l(r, \mathcal{E}_1)$ is not deformed at all.

Apart from a better description of eigenfunctions close to \mathcal{E}_1 , the setup of matrix elements is faster using APW + lo compared to LAPW, since a majority of the basis functions include only u_l .

2.2. The kinetic energy operator

The APW + lo and LAPW methods differ in a second, important way. While the augmentations in LAPW are smoothly connected to the plane waves, there is no restriction on the derivatives of the APW + lo basis functions at the MT boundaries.

The Laplacian operator is commonly used to describe the

kinetic energy $\int_V \phi_{\mathbf{G}}^*(-\nabla^2)\phi_{\mathbf{G}'} dV$ although the formulation using nabla operators $\int_V (\nabla\phi_{\mathbf{G}})^\dagger \cdot \nabla\phi_{\mathbf{G}'} dV$ is more fundamental, as it enters already in the variational principle leading to the Schrödinger equation [1,13]. According to Green's theorem the two kinetic energy expressions differ by an integral:

$$\oint_{S_{\text{MT}}} \phi_{\mathbf{G}}^* \left(\frac{\partial \phi_{\mathbf{G}'}^{\text{MT}}}{\partial r} - \frac{\partial \phi_{\mathbf{G}'}^{\text{I}}}{\partial r} \right) dS. \quad (6)$$

It is clearly seen that this surface term vanishes in LAPW, where the functions $\phi_{\mathbf{G}}$ have continuous derivatives on the MT spheres S_{MT} . However, using the APW + lo basis functions, this term must be taken into account whenever the Laplacian operator is used to represent the kinetic energy:

$$T_{\mathbf{G}\mathbf{G}'} = \int_{\text{I}+\text{MT}} \phi_{\mathbf{G}}^*(-\nabla^2)\phi_{\mathbf{G}'} dV + \oint_{S_{\text{MT}}} \phi_{\mathbf{G}}^* \left(\frac{\partial \phi_{\mathbf{G}'}^{\text{MT}}}{\partial r} - \frac{\partial \phi_{\mathbf{G}'}^{\text{I}}}{\partial r} \right) dS. \quad (7)$$

Or, as the nabla operator is more convenient in the interstitial region,

$$T_{\mathbf{G}\mathbf{G}'} = \int_{\text{I}} (\nabla\phi_{\mathbf{G}})^\dagger \cdot \nabla\phi_{\mathbf{G}'} dV + \int_{\text{MT}} \phi_{\mathbf{G}}^*(-\nabla^2)\phi_{\mathbf{G}'} dV + \oint_{S_{\text{MT}}} \phi_{\mathbf{G}}^* \frac{\partial \phi_{\mathbf{G}'}^{\text{MT}}}{\partial r} dS. \quad (8)$$

A different approach, starting from the Laplacian operator is adapted by Schlosser and Marcus [14]. They then have to modify the variational expression, taking into account the discontinuity in slope at the MT sphere, but end up with the same expression, Eq. (7) for the kinetic energy operator.

3. Results

The flexibility of a basis set can be appreciated by looking at how well a smaller number of basis functions reproduce the final, converged total energy. The APW + lo and LAPW methods are run self-consistently for an increasing plane-wave cut-off, G_{max} . All calculations in this paper are full-potential calculations, using a scalar relativistic approximation and the Hedin–Lundqvist [15] version of the local density approximation to the density-functional theory [5].

The first trial system is fcc copper, and thereafter we turn to fcc cerium, where extra treatment of extended-core states is required. The calculations for copper and cerium are performed using the experimental lattice constants $a = 6.82$ and $a = 9.05$ a.u., respectively. The effects on the matrix dimensions from a reduced G_{max} are larger for an

Table 1

Number of plane-waves corresponding to different $r_{\text{MT}}G_{\text{max}}$. A random \mathbf{k} -point = $2\pi/a(0.1875, -0.625, 0.3125)$ is used for fcc Cu ($r_{\text{MT}} = 2.35$ a.u.) and fcc Ce ($r_{\text{MT}} = 3.14$ a.u.). The Γ -point is used for O₂ ($r_{\text{MT}} = 1.00$ a.u.)

$r_{\text{MT}}G_{\text{max}}$	Number of plane-waves		
	Cu	Ce	O ₂
3.0	–	–	285
5.0	14	14	1335
7.0	36	35	3663
9.0	77	76	6979
11.0	139	137	–
13.0	224	219	–
15.0	334	335	–

open structure, and so the third system is chosen to be an oxygen molecule in a supercell approximation. The Brillouin zones of copper and cerium are represented by 60 special \mathbf{k} -points, while the small Brillouin zone of the oxygen molecule in a supercell is treated using only the Γ -point. The plane-wave cut-off is conveniently expressed by the dimensionless product of the MT-radius, r_{MT} and the largest reciprocal lattice vector used in the plane wave expansion, G_{max} . The exact number of plane-waves corresponding to a certain $r_{\text{MT}}G_{\text{max}}$ is \mathbf{k} -point dependent, but Table 1 shows the correspondence for a random \mathbf{k} -point in the Brillouin zones of Cu and Ce, and for the Γ -point of the O₂ molecule. On an average the size of the basis set for a fixed r_{MT} , is proportional to G_{max}^3 .

3.1. Copper

APW + lo uses complementary local orbitals for $l = s, p$ and d , which renders nine extra basis functions to be added

to the number of plane-waves in Table 1. Fig. 3 shows that APW + lo reaches the final total energy (within 1 mRy) for $r_{\text{MT}}G_{\text{max}} = 9$, corresponding to approximately 75 + 9 basis functions, while LAPW needs $r_{\text{MT}}G_{\text{max}} = 10$ which gives about 100 basis functions.

The two methods converge to numerically the same densities and total energies as well as individual eigen-energies. These values do not coincide for finite basis sets as the basis functions in the MT region in the two methods consist of *differently constrained* combinations of u_l and \dot{u}_l .

3.2. Cerium

The local orbitals described in Section 2 are not suited for treating semi-core states. In Ref. [12] Singh introduces local orbitals containing radial solutions u_l evaluated at lower linearization energies. The same thing can be done for APW + lo, using a *second kind* of local orbitals, with $R_L^{l0}(r) = a_L^{l0}u_l(r, \mathcal{E}_1) + c_L^{l0}u_l(r, \mathcal{E}_2)$. The energy parameter \mathcal{E}_2 is chosen so that $u_l(r, \mathcal{E}_2)$ is optimized for describing the extended-core states. a_L^{l0} can be chosen arbitrarily while c_L^{l0} is found by requiring $\phi_L^{l0} = 0$ at the MT boundary, as before.

The APW + lo basis set is constructed with the first kind of local orbitals for $l \leq 3$, as the behavior of the cerium 4f-states is critical for the resulting energy. The second kind of local orbitals, including $u_l(r, \mathcal{E}_2)$, are used to treat the high lying 5s and 5p core states in cerium. In the LAPW method, the semi-core states of s and p are treated by local orbitals as described in Ref. [12]. As for copper, APW + lo shows (Fig. 4) a faster convergence than LAPW in terms of $r_{\text{MT}}G_{\text{max}}$. While APW + lo obtains the final total energy (within 1 mRy) for $r_{\text{MT}}G_{\text{max}} = 9$, giving around 75 + 20 basis functions, LAPW uses $r_{\text{MT}}G_{\text{max}} = 10$, corresponding to about 100 + 4 basis functions when reaching the same accuracy.

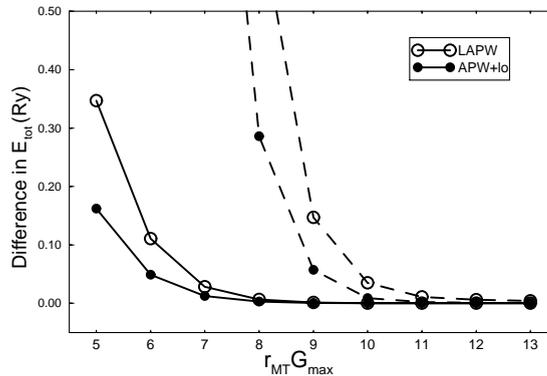


Fig. 3. Convergence of total energy versus $r_{\text{MT}}G_{\text{max}}$ for Cu ($r_{\text{MT}} = 2.35$ a.u.). The solid lines correspond to the values of the energy axis, while the dashed lines show the values multiplied by 100. The APW + lo energy for $r_{\text{MT}}G_{\text{max}} = 13$ is used as reference energy.

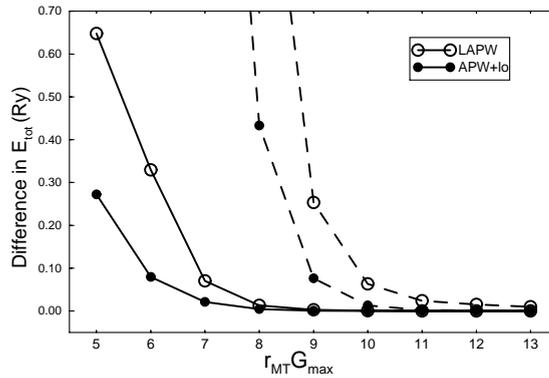


Fig. 4. Convergence of E_{tot} versus $r_{\text{MT}}G_{\text{max}}$ for Ce ($r_{\text{MT}} = 3.14$ a.u.). The energy differences (solid lines) are also shown enhanced by 100 (dashed lines). The reference energy is taken to be the APW + lo energy for $r_{\text{MT}}G_{\text{max}} = 13$.

3.3. Oxygen molecule

The oxygen molecule vibrates about its equilibrium bond length R_e , with a vibrational frequency $\nu_e \propto (d^2E/dR^2)|_{R_e}$. The bond length and corresponding vibrational frequency are obtained from LAPW and APW + lo as functions of increasing $r_{\text{MT}}G_{\text{max}}$.

A tetragonal unit cell with $a = 8.0$ and $c = 10.0$ a.u. is used with the oxygen molecule directed along the c -direction. A small MT-radius, $r_{\text{MT}} = 1.0$ a.u., is required due to the short bond length. The calculations are spin-polarized to allow for the triplet ground state. The APW + lo basis set includes local orbitals for $l = s$ and p , i.e. four extra basis functions per atom for each spin. As seen in Fig. 5, APW + lo yields a bond length R_e within 1.1% of the final result for $r_{\text{MT}}G_{\text{max}} = 4.0$, corresponding to 685 + 8 basis functions per spin, while LAPW demands at least $r_{\text{MT}}G_{\text{max}} = 5.5$ giving 1773 basis functions per spin for

the same accuracy. The vibrational frequency ν_e converges slower for the two methods, but APW + lo again approaches its final result much faster than LAPW. For an accuracy within 5% of the final value APW + lo uses $r_{\text{MT}}G_{\text{max}} = 4.5$, giving 821 + 8 basis functions per spin, whereas LAPW needs $r_{\text{MT}}G_{\text{max}} = 5.5$, corresponding to 1773 basis functions per spin.

APW + lo also converges towards its final values in a smoother way than LAPW. Thereby even a crude APW + lo calculation gives good approximate values. Lowering the number of basis functions by around 1000 yields a substantial reduction in computational cost. Standard matrix diagonalization routines, as are commonly used in LAPW and APW codes, have computational times that scale with the cube of the number of basis functions and the required memory scales with the square.

Our calculations are in fair agreement with the experimental

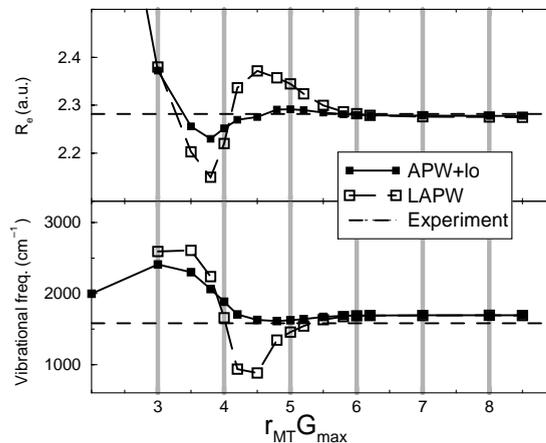


Fig. 5. Convergence in vibrational frequency ν_e with respect to $r_{\text{MT}}G_{\text{max}}$ for O_2 . Experimental $\nu_e = 1580 \text{ cm}^{-1}$. Convergence in equilibrium bond length R_e with respect to $r_{\text{MT}}G_{\text{max}}$ for O_2 . Experimental $R_e = 2.28$ a.u.

values [16] for the oxygen molecule, $R_e^{\text{Exp}} = 2.28$ a.u. and $\nu_e^{\text{Exp}} = 1580 \text{ cm}^{-1}$, as well as with other density functional calculations [17]. However, for a detailed comparison, convergence with respect to the size of the unit cell should be examined more carefully. This has not been done here, as the main purpose is to compare the two theoretical methods.

4. Conclusions

The results of Section 3 indicate that it is more efficient to introduce extra radial solutions, such as \dot{u}_l via local orbitals rather than into the ordinary basis functions. The latter way imposes additional restrictions on the basis set which in turn demands a larger number of basis functions. This is in accordance with the results of Ref. [12], where LAPW + lo converges faster than the methods having continuous second and third derivatives, SLAPW-3 and SLAPW-4, respectively. The fact that APW + lo in practice converges to the same total energy, and the same individual eigenvalues, as does LAPW is important. A kink in the eigenfunctions would alter the kinetic energy, due to the surface term in Eq. (6). We can therefore be sure that the final, converged eigenfunctions are differentiable everywhere, as required for physical meaningfulness.

The two basis sets, APW + lo and LAPW consist of the same functions u_l and \dot{u}_l and could easily be mixed in the same code. For example, calculations for a molecular reaction on a metal surface could be performed with an APW + lo basis set for the adsorbate and a well-tested LAPW treatment for the substrate.

Due to the smaller basis set and faster matrix set up, APW + lo offers a shorter run-time and uses less memory than LAPW. The effects of using APW + lo are greatest for calculations with a large ratio of basis functions to atoms, e.g. for open crystal structures, surfaces and molecules on surfaces.

Acknowledgements

We are grateful to Stefan Blügel for useful discussions, and for encouraging the presentation of this work within the FLAPW-node of the TMR-network. Discussions with Peter Blaha concerning a mixed APW + lo and LAPW basis set are acknowledged. Using the oxygen molecule as a trial system for the APW + lo method was suggested by Raimund Podloucky.

E.S. and L.N. acknowledge the financial support from the Swedish Natural Science Research Council, while the work by D.J.S. is supported by the Office of Naval Research.

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