



# Core Boundary Conditions in the Full-Potential LMTO Code LMF

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# Core Boundary Conditions in the Full-Potential LMTO Code LMF

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**Abstract** –The accuracy of alternative core treatments in relativistic density functional theory calculations is discussed for the full-potential linearised-muffin-tin-orbital code `lmf`. Atomic solutions are compared with reference data and HCP titanium is used as a representative band problem, where results are compared with those obtained using the full-potential augmented plane-wave code `fleur`. Self-consistent update of the core density is shown to be less important than the correct incorporation of charge leaking from the core into the interstitial.

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**Introduction.** – Modern approaches to solving the electronic structure problem for crystalline materials distinguish between core and valence states. Different numerical techniques are applied for the solution of the tightly bound core states and for the valence states, which participate in band formation. Because the core states only indirectly influence band formation, they frequently receive more approximate treatment than the valence states. The various *pseudopotential* schemes model the effect of the nucleus and core states by an effective, but *l*-dependent, potential with the corresponding pseudo-wave functions are essentially smooth in space and easily represented by a small plane-wave basis.

*Augmented* methods, which rely upon Slater's muffin-tin decomposition of space between atomic spheres and interstitial, allow the simultaneous solution of the core and valence states and are often called *all-electron* methods. There is a variety of all-electron methods differing principally in the basis and in the representation of the potential and density. The highest level of accuracy is only afforded by those methods which are capable of describing faithfully the variation of the potential and density in the interstitial: these are the *full-potential* all-electron methods, which are the subject of this Report.

Modern full-potential all-electron schemes rely upon Andersen's linearisation [1], which means that the band problem is accurately solved only within a certain energy range ( $\sim$ Hartree around the Fermi level). Core states lie well beyond this energy range and to allow their description on the same footing as valence states, while possible in principle, would require having several such *windows*, a significant increase in complexity. Instead core states are often solved under the simplifying assumptions that they do not participate in bonding and that they experience a central potential. The core problem thereby becomes a radial problem with fixed boundary conditions which is easily solved. The core density can be evaluated and used in the calculation of the potential experienced by the valence states; approximate orthogonality of the valence states to the core states is afforded by the correct nodal structure of the valence states in the augmented methods. The core states (density) may be determined once and for all in an atomic calculation or may be updated self-consistently during the solution of the crystal problem.

This Report discusses the effects of different core electron treatment choices in high accuracy total energy calculations for solids in the framework of density functional theory. The specific core treatment options considered are the use of the *frozen* atomic core density or the self-consistently updated density in the spherical component of the crystal potential, whether or not to allow the core density to extend into the interstitial region, and the effect of including some core states in the valence set explicitly. This latter possibility is allowed in both of the tested codes by the use of *local orbitals*.

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<i>core</i>	radial Dirac equation	rel. LDA/VWN	spherical potential
<i>valence</i>	within $r_{mt}$ : radial Pauli equation ( <i>scalar-relativistic</i> ) interstitial: non-relativistic	rel. LDA/VWN	full potential

Table 1: Description of the relativistic local density approximation (RLDA) used in this Report for the core, augmentation and interstitial parts in the LMTO/APW methods. In these methods, the *basis* within the augmentation region is calculated within the spherical part of the crystal potential; this basis is then used to express solutions to the *full* potential problem.

### Computational Details. –

*HCP Titanium.* HCP titanium at the experimental lattice structure ( $a = 2.95111\text{\AA}$ ,  $c/a = 1.5873$  [2]), is chosen as a simple test case; the 3p state is relatively shallow in titanium and its inclusion in the core or valence can be used to illustrate the effect of the core state boundary conditions. As a light element, the effects of relativity in titanium can be expected to be small (calculations below show what small means in this context). Although there are few core states in titanium, the essential complexity of the problem is common to all the non-magnetic elemental d-block materials. The typical division for titanium is core:  $1s^2, 2s^2, 2p^6, 3s^2, 3p^6$  (18 electrons) and valence:  $4s^2, 3d^2$ . High quality LAPW calculations for titanium were first presented 30 years ago by Lu, Singh and Krakauer [3].

*FP-LMTO and FP-LAPW Codes.* The two full-potential all-electron codes are **fleur** [4, 5] (version “Max-release 1.3”), which is an implementation of the linearised augmented plane wave (LAPW) method, and **lmf** [6, 7] (version “7.11.j”, build ref: f2a1c5c) which is based on the linearised muffin-tin orbital (LMTO) technique.

The LAPW and LMTO methods both separate space into non-overlapping spherical regions surrounding the nuclei, *muffin-tin* or *augmentation spheres* with radius  $r_{mt}$ , and the remaining interstitial region. The single-particle Schrödinger equation is then solved separately in these two regions, with solutions that are matched at  $r_{mt}$ . The boundary of the augmentation sphere radius also represents the limit of outwards integration of the core states. The total energies calculated by the LAPW and LMTO schemes are (differently) sensitive to  $r_{mt}$ , which must be chosen by the user. In order to allow a detailed comparison of total energies, identical  $r_{mt}$  are chosen with value 2.65Bohr. This is a typical choice for LMTO calculations, being somewhat smaller than the touching sphere radius and so maximising the volume of the augmentation region: here the quality of the solution is expected to be better than in the interstitial. This concern is particularly applicable to the LMTO method, which relies on an almost minimal basis for the interstitial.

For the purposes of this comparison, three modifications to **lmf** have been made to increase the core grid limits in some subroutines, to enable the use of relativistic exchange in **libxc** and to activate the Dirac solver in the self-consistent case. These developments will be available in a forthcoming release.

*Relativistic Local Density Approximation.* Scalar-relativistic solvers – which include relativistic effects in the kinetic energy except the spin-orbit term (see [8] for discussion and [9] for implementation considerations) – are used consistently in the codes for the valence calculations. **lmf** features both scalar- and fully-relativistic (Dirac) core solvers; in **fleur** only the Dirac solver is implemented. The local density approximation is used for exchange and correlation as parameterised by Vosko, Wilk and Nussair [10]. Relativistic effects are not usually included in the exchange correlation functional, but doing so (in the framework of MacDonald and Vosko [11]) allows for direct comparison with high precision reference data. In the **lmf** code, the relativistic correction to exchange is provided by the **libxc** library [12]. The combined use of the Dirac core solver and relativistic density functional is referred to here as *relativistic local density approximation* (RLDA).

While **lmf** and **fleur** codes were developed independently and many implementation details are different, both codes have adopted the same radial meshing for the augmentation region:  $r_i = r_0(\exp(a(i-1)) - 1)$ , for grid points  $i = 1..n$ . The radial mesh is specified by the number of points,  $r_{mt}$  and the parameter  $a$ . The best meshing possible in **lmf** is with  $n = 1473$  (the limit is 2000) and  $a = 0.0065$ . This has been used in both codes for convenience of plotting the core density. Tests with **fleur** show that for this choice of radial grid the total energy (in the crystal case) is within  $25\mu\text{Hartree}$  of the converged result.  $\vec{k}$  is sampled in both codes using a Monkhorst-Pack grid of  $28 \times 28 \times 15$  (640 points in the irreducible wedge), which is sufficient for 1  $\mu\text{Hartree}$  convergence. For **lmf** an *spdf/spd* MTO basis was used with Hankel energies and spearing widths chosen automatically, combined with  $l_{max} = 4$  augmentation. The specific basis definitions are given in listing2. **fleur** calculations employ a  $K_{max} = 3.7$  ( $G_{max} = 10\text{Bohr}^{-1}$ ) and augmentation cutoff  $l_{max} = 10$ . Sample **lmf**

and `fleur` inputs are provided in listings 1,3.

**Atomic Problem.** – Table 2 compares the `lmf` core eigenvalues and total energy with high quality reference data in the RLDA formalism for the case of atomic titanium provided by Kotochigova, Levine, Stiles and Clark at NIST [11]. The agreement of core eigenvalues and the total energy are better than 1mHartree; this suggests that energies larger than this can be considered accurate.

	<code>lmf</code>	NIST [13]
1s	-178.025331	-178.025322
2s	-19.642807	-19.642824
2pM	-16.439494	-16.439503
2pP	-16.228617	-16.228623
3s	-2.284593	-2.284637
3pM	-1.441010	-1.441054
3pP	-1.416620	-1.416663
$E_{total}$	-851.162158	-851.162463

Table 2: Atomic Ti core eigenvalues calculated using `lmf` compared with standardised data for the solutions of the radial Dirac equation with relativistic LDA exchange-correlation [11] (RLDA). “P” denotes  $j = l + 1/2$ , “M” for  $j = l - 1/2$ . Units are Hartree. Radial mesh parameter  $a = 0.0065$ .

The total energy is also listed; note that in `lmf` the valence 4s and 3d states do not include the spin-orbit interaction (they are *scalar-relativistic*), while the NIST reference data is entirely within Dirac formalism. This gives rise in this case to no significant error in the calculated total energy. `lmf` calculates the amount of charge of each state beyond  $r_{mt}$ ; here the *leakage* is negligible except for the 3s state,  $q(r > r_{mt}) = 0.00143e/\text{atom}$  and 3p, where each state leaks  $q(r > r_{mt}) = 0.00557e/\text{atom}$ .

### Solid State Calculations. –

*Frozen Overlapping Core Approximation.* The simplest scheme is to include the core density from a free atom calculation directly and without modification in the band calculation. The core density is added to the valence density when calculating the Hartree and exchange-correlation energies and potentials. If the free atom core density is allowed to extend into the interstitial and overlap with that of other atoms when the crystal is formed, this additional density must also be included in the interstitial problem. This *frozen overlapping core approximation* (FOCA) is implemented in the `lmf` code. The core density, which is also spherically symmetric, is fitted in `lmf` to a Hankel function with  $l = 0$ : beyond  $r_{mt}$ , atomic wave functions die away exponentially and a single smoothed Hankel function is an appropriate fit (see fig. 1). Details can be found in the NFP Manual by M. Methfessel (October 10,1997), which documents an earlier version of the `lmf` code [14]. The default smoothing radius for the representation of the core density tail is used (1.06bohr); this small value corresponds to a very weakly smoothed Hankel function.

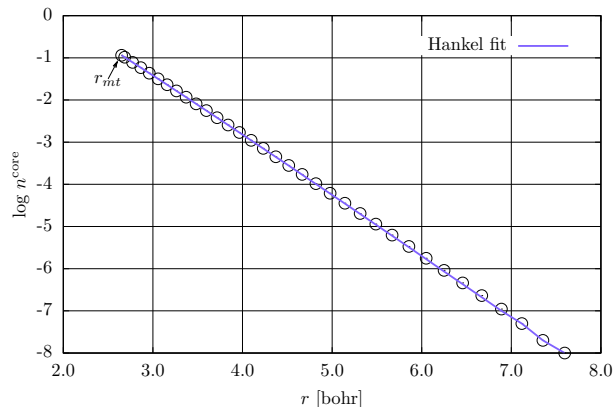


Fig. 1: Atomic Ti core density beyond  $r_{mt} = 2.65\text{Bohr}$  and corresponding  $l = 0$  Hankel fit, RLDA as calculated using `lmf`.

*Self-consistent Core.* Because core states are energetically deep and localised close to the nucleus of the atom, where the potential landscape is dominated by the nuclear potential, it has proven reliable to replace the full potential by its spherically symmetric component. For the valence states, the potential within the muffin-tin sphere is typically expanded by angular momentum, and it is therefore a straightforward task to provide the spherical part to be used in evaluation of the core states. An important caveat is that the potential is expanded by  $l$  in this way only within the augmentation sphere: there is no obvious radial tabulation of  $V$  for  $r > r_{mt}$ . Accordingly, the choice is often made to require core wave functions and their first derivatives to be zero at  $r_{mt}$ . This choice is made in `lmf` when self-consistent core treatment is chosen by the user.

The `fleur` implementation addresses this difficulty by extrapolating the potential beyond  $r_{mt}$  using a simple quadratic function determined by the value of the potential at the muffin tin boundary (the potential is shown in fig.2). The core states are obtained as solutions to this extrapolated potential and any charge beyond  $r_{mt}$  can be included (either using Hankel tails up to  $lmax = 6$ , or simply averaged over the interstitial volume) in the interstitial density. Some discussion about the form of the potential for  $r > r_{mt}$  may be found in Zabludil et al.'s, treatise [15].

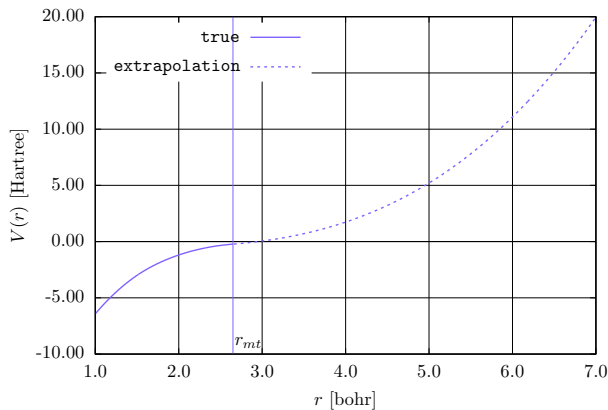


Fig. 2: Extrapolation of the core potential beyond  $r_{mt}$  in `fleur` to form a quadratic confining potential.

The RLDA core eigenvalues calculated self-consistently in the crystal case are presented in table 3, where differences in the summed core eigenvalues and kinetic energies are seen in the mHartree range.

	<code>lmf</code>	<code>fleur</code>
1s	-177.799011	-177.800568
2s	-19.423005	-19.423376
2pM	-16.218969	-16.219412
2pP	-16.008128	-16.008562
3s	-2.060614	-2.059892
sum T core	805.5763	805.5772
sum $e_i$ core	-495.0357	-495.0407

Table 3: Ti core eigenvalues self consistently calculated in the crystalline environment. RLDA: “P” denotes  $j = l + 1/2$ , “M” for  $j = l - 1/2$ ,  $e_i - e_F$  are tabulated in Hartree. In `lmf` the self-consistent core mode is selected by setting `LFOCA=0`.

*Local Orbitals for Semi-core States.* When it is questionable whether some atomic state should be treated as core, it may be additionally included in the valence using local orbitals (LO) [16]. In the *conventional* implementation, local orbitals are solutions to the radial problem that are constructed to be only non-zero within the augmentation sphere. These functions are added to the basis within the augmentation region and allow, in combination with the usual valence augmentation, the additional description of states with different quantum number, for some  $l$ . Depending upon construction of the local orbital, it can be used to describe semi-core states (with lower quantum number) or unoccupied states (by using a higher quantum number in setting up the local orbital). *Conventional* local orbitals use the same basis functions in the interstitial as the main valence band. In LMTO, the basis functions (smoothed Hankel functions) are optimal for the valence

band and are poor in describing deeper semi-core states and it is advantageous to form *extended* local orbitals, where additional Hankel functions are fitted to match the local orbital in value and gradient at  $r_{mt}$ .

*Total Energy Comparison.* The HCP total energies at the experimental lattice constant are given in table 4. The `fleur` code, in which the core density is always allowed to extend into the interstitial, shows particularly

<i>code</i>	<i>method</i>	$q_{\text{core loss}}$	$E_{\text{total}}$ [Hartree/at]
<b>lmf</b>	<i>scf core, constrained to <math>r_{mt}</math></i>	0	-851.460199
	<i>scf core, constrained to <math>r_{mt}</math>, 3p-LO(conventional)</i>	0	-851.431693
	<i>scf core, constrained to <math>r_{mt}</math>, 3p-LO(extended)</i>	0	-851.436017
	<i>frozen core, overlapping tail</i>	0.0363	-851.434890
	<i>frozen core, overlapping tail, 3p-LO(conventional)</i>	0.0029	-851.430236
	<i>frozen core, overlapping tail, 3p-LO(extended)</i>	0.0029	-851.434559
<b>fleur</b>	<i>scf core, tail averaged in interstitial</i>	0.0430	-851.434720
	<i>scf core, overlapping tail</i>	0.0431	-851.434789
	<i>scf core, overlapping tail, 3p-LO(conventional)</i>	0.0032	-851.434657

Table 4: Total RLDA energies for HCP titanium for different core treatments.

consistent total energies when calculated with different core options. The use of the confining potential for treating the core states is justified by the close agreement with the results obtained by explicit inclusion of the 3p core states in the valence. The `lmf` results calculated with self-consistent core treatment – which implies that the core states are restricted to  $r_{mt}$  – differ significantly, while the overlapping frozen core treatment gives results in much closer agreement with the `fleur` calculations. When the 3p states are included in the valence, either using conventional or extended local orbitals, the agreement between `lmf` results with self-consistent and frozen cores is much improved, although a difference of 1.5mHartree persists. When extended local orbitals are used in `lmf`, the agreement with `fleur` is much improved compared to the use of conventional local orbitals. The difference in the core loss between `lmf` and `fleur` ( $0.036e/at$  compared with  $0.043e/at$ ) suggests that the 3p states extend more into the interstitial (i.e. beyond  $r_{mt}$ ) in the crystal case than in the atomic limit – consistent with some hybridisation of the 3p states.

*Equation of State.* At fixed  $c/a$ , the total energy is calculated for cell volumes between 224.6 and 218.5Bohr<sup>3</sup> allowing Birch-Murnaghan equation of state parameters to be calculated (table 5). Muffin-tin spheres almost touch at the smallest volume and basis parameters are unchanged for all volumes. The `lmf` calculations show some scatter, in particular the self-consistent core gives an outlying estimate of the lattice constant. The frozen core results with and without 3p local orbitals are in better agreement. Although the range of minimum energies is smaller in `fleur`, the bulk modulus clearly depends upon the inclusion of 3p LO. The `fleur` and `lmf` results including the 3p LO with overlapping core tails are in very good agreement. Because these setups may be considered to be the best in that they have the largest basis (and so variational freedom), and because they show consistent agreement, it is reasonable to interpret these results as the most accurate RLDA description. The extremely good agreement of these calculations show that the core relaxation, which is present in `fleur` but not the `lmf` calculations, is of negligible importance here. It is not clear why the overlapping tail without LO in `fleur` deviates more than the corresponding `lmf` calculation.

<i>code</i>	<i>method</i>	$E(V_0)$ [Hartree/at]	$a_0$ [Bohr]	$B_0$ [GPa]
<b>lmf</b>	<i>scf core, constrained to <math>r_{mt}</math></i>	-851.462383	5.3898	118.6
	<i>frozen core, overlapping tail</i>	-851.436255	5.4379	132.9
	<i>frozen core, overlapping tail, 3p-LO(extended)</i>	-851.436116	5.4274	130.9
<b>fleur</b>	<i>scf core, tail averaged in interstitial</i>	-851.436776	5.3966	119.5
	<i>scf core, overlapping tail</i>	-851.436951	5.3904	117.4
	<i>scf core, overlapping tail, 3p-LO(conventional)</i>	-851.436132	5.4320	132.5

Table 5: Calculated RLDA HCP titanium lattice parameter, minimum energy and bulk modulus for different core treatments with fixed  $c/a = 1.5873$ .

*Effect of Relativity.* The different treatment of relativity for the core is significant for total energy comparisons but gives only small changes to the equilibrium lattice parameters (the bulk-modulus is more sensitive).

The scalar-relativistic treatment is inferior to the full Dirac treatment because the spin-orbit interaction is significant for the core states and does cause a change in the core density. The use of the relativistic variant of the LDA gives rise to significant differences to the total energy; these are larger than the differences between using the Dirac equation or the simpler scalar relativistic equations for the core solver. Whether or not to use relativistic corrections to the exchange-correlation functional is an open question since the theory of current-density functional theory remains incomplete.

	$E(V_0)$ [Hartree/ $at$ ]	$a_0$ [Bohr]	$B_0$ [GPa]
RLDA	-851.436116	5.4274	130.9
scalar core, relativistic LDA	-851.428497	5.4274	109.9
scalar core, usual (non-rel.) LDA	-852.007063	5.4266	109.8

Table 6: Calculated HCP titanium lattice parameter with fixed  $c/a = 1.5873$  for different models for relativity. Calculations using `lmf` with frozen overlapping core and 3p-LO(extended).

### Conclusions. – The Report:

1. illustrates the relatively minor role of self-consistency in the core compared with inclusion of core density in the interstitial
2. demonstrates that agreement in the total energy better than mHartree is possible between the codes tested, when each is well converged
3. shows that different treatment of relativity in the core leads to energy differences greater than 1mHartree, even in titanium where this would not be expected
4. verifies `lmf`'s core eigenvalues against robust reference data
5. shows that the spatial distribution of leaked core charge in the interstitial is less significant than the amount of leaked charge: a uniform distribution is of quality comparable to an  $l$ -expansion of Hankel functions
6. confirms that the current `lmf` frozen core implementation is adequate for accurate calculations
7. shows the utility of local orbitals for improving the treatment of semi-core states; in `lmf` extended local orbitals should be strongly preferred over the conventional type.

Here *good* is understood to mean *agreement of total energy better than 1mHartree*.

The response of the core to changes in the valence states should be considered only for high-accuracy calculations, but at present this is prevented in `lmf` by the loss of accuracy incurred by the boundary conditions. The close agreement of `fleur` results with self-consistent core and LO methods suggests that the inclusion of a confining potential (or alternative means of extending the core integration beyond  $r_{mt}$ ) is necessary for self-consistent core calculations, but, when this is done, that such core schemes do allow very high accuracy.

The use of extended local orbitals in `lmf` is recommended for semi-core states such as the 3p in Ti whenever high accuracy is required. A working definition of semi-core corresponds to those states deeper than  $\sim -1.25$  Hartree in the atomic problem, or where the charge corresponding to the state beyond  $r_{mt}$  exceeds 0.002e; these are inclusive criteria but, wherever there is doubt, testing should confirm whether or not the inclusion of the semi-core state affects the calculated properties.

\* \* \*

Assistance in setting up local orbitals in `fleur` is gratefully acknowledged from Gregor Michalicek, FZ Jülich.

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Listing 1: lmf control file (3pLO will be added automatically because of the LOC=1 flag)

```

1  VERS LMF=7 LM=7 FP=7
2  IO  VERBOS=60
3  % const gmax=10.0 # L0 case
4  HAM
5  AUTOBAS [LMT0=5 MTO=2 LOC=1] # spdf/spd MTO basis with L0
6  GMAX={gmax}
7  XCFUN=0 001 007 # VWN via libxc
8  TOL=1e-16
9  REL=11 # Dirac core
10 BZ
11 % const nk=-12000
12 NKABC={nk}
13 METAL=5
14 EWALD
15 TOL=1e-16
16 ITER
17 NIT=30
18 CONV=1e-7
19 MIX[B8,b=1.0]
20 SYMGRP find
21 STRUC
22 NBAS=2 NSPEC=1
23 ALAT=5.57682 # RT, atmospheric ICSD 43416, a=2.95111A,c/a=1.5873
24 PLAT=1 0 0 1/2 sqrt(3)/2 0 0 0 1.5873
25 SPEC
26 # lfoca=1 for frozen core, lfoca=0 for self consistent core
27 % const lmx=3 lmx=6 a=0.0065 lfoca=1
28 ATOM=Ti Z=22 R=2.65 LMX={lmx} LMXA={lmxa} A={a} LFOCA={lfoca}
29 SITE
30 ATOM=Ti XPOS=0.0000000 0.0000000 0.0000000
31 ATOM=Ti XPOS=0.3333333 0.3333333 0.5000000

```

Listing 2: lmf smoothed Hankel basis definitions)

```

1  BASIS:
2  Ti RSMH= 1.767 1.767 1.234 1.767 EH= -0.1 -0.1 -0.1 -0.1 RSMH2= 1.767 1.767 1.234 EH2= -0.9 -0.9 -0.9 PZ= 0 13.9377

```

Listing 3: fleur control file with explicit 3pLO

```

1  <?xml version="1.0" encoding="UTF-8" standalone="no"?>
2  <fleurInput fleurInputVersion="0.27">
3    <comment>
4      Ti core study, setup 1
5    </comment>
6    <calculationSetup>
7      <cutoffs Kmax="3.7" Gmax="10.0" GmaxXC="6.0" numbands="0"/>
8      <scfLoop itmax="20" maxIterBroyd="99" imix="Broyden2" alpha="0.4" spinf="1.0"/>
9      <coreElectrons ctail="T" frcor="F" krel="0"/>
10     <magnetism jspins="1" l_noco="F" swsp="F" lflip="F"/>
11     <bzIntegration valenceElectrons="20.0" mode="hist" fermiSmearingEnergy="0.0005">
12       <kPointMesh nx="28" ny="28" nz="15" gamma="F"/>
13     </bzIntegration>
14     <energyParameterLimits ellow="-1.0" elup="1.0"/>
15   </calculationSetup>
16   <cell>
17     <symmetryFile filename="sym.out"/>
18     <bulkLattice scale="1.0" latnam="hex">
19       <a1>5.57682</a1>
20       <c>8.852086</c>
21     </bulkLattice>
22   </cell>
23   <xcFunction name="vwn" relativisticCorrections="T"/>
24   <atomSpecies>
25     <species name="Ti-1" element="Ti" atomicNumber="22" coreStates="5" magMom="0.0" flipSpin="F">
26       <mtSphere radius="2.65" gridPoints="1473" logIncrement="0.0065"/>
27       <atomicCutoffs lmax="10" lnonsphr="6"/>
28       <energyParameters s="4" p="4" d="3" f="4"/>
29       <lo type="SCL0" l="1" n="3" eDeriv="0"/>
30     </species>
31   </atomSpecies>
32   <atomGroups>
33     <atomGroup species="Ti-1">
34       <relPos>1.0/3.0 1.0/3.0 1.0/4.0</relPos>
35       <relPos>-1.0/3.0 -1.0/3.0 -1.0/4.0</relPos>
36     </atomGroup>
37   </atomGroups>
38 </fleurInput>

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