

Ψ_k - NEWSLETTER

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on Electronic Structure of Solids

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CCP9 NEWSLETTER

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What is the CCP9 and how to use it

B.L. Gyorffy, Chairman of the Working Group

The Computer Board of the Science and Engineering Research Council funds Computational Collaborative Projects (CCP) with the aim of encouraging collaborations on projects involving large scale calculations and aiding rapid dissemination of computational 'know-how' in various areas of Physics and Chemistry (Quantum Chemistry, Surface Science etc.). The CCP-9 has been established to help those of us, in the condensed matter physics community, whose work involves calculations of the electronic structure. For arguments in support of our application see our previous " ψ_k -newsletter".

What we have is: a) some money (£3500) for travel to collaborate and for organizing one day meetings, b) funds for a research assistant (RA) who will act as a catalyst and our secretary, c) possibilities for inviting Senior Visiting Fellows (SVF), d) and some time allocation on the Cray IS computer at Daresbury. The tenure of this grant is to be three years.

Temporarily, Dr. Walter Temmerman of the Band Theory Project at Daresbury is acting as our secretary. The RA position will be advertised shortly. (Suggestions are welcomed and should be sent to me.) Our first SVF is Dr. G.M. Stocks of the Oak Ridge National Laboratory (USA) and he is already at Daresbury.

At our one day meeting in November (see elsewhere in this Newsletter) it was decided that CCP9 would be run by the Working Group which would report to the membership annually at a similar one-day meeting (see announcement of our symposium in London, Dec. 1982). The Working Group consists of spokesmen from each project. It meets twice a year to review current projects and accept new ones. What constitutes a collaborative project is not defined rigidly but the description of the

first batch, approved by the WG at its first meeting, overleaf, should give a clear idea of what we have in mind. Anyone wishing to propose a new project should get in touch with Walter or me. The next meeting of the WG will be at the EPS conference in Manchester.

Self-consistent-field calculations of the electronic structure of
 $\text{Ag}_{1-c}\text{Pd}_c$ random alloys*

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H. Winter, Kernforschungszentrum Karlsruhe, West Germany.

When used in conjunction with a general muffin-tin description of the crystal potential function, the coherent-potential-approximation (CPA)¹ provides an accurate and detailed understanding of a wealth of experimental information on the electronic structure of random metallic alloys^{2,3}. Currently the only inputs to these first principles (KKR-CPA)^{2,4} calculations are the crystal structure and lattice spacing of the alloy in question together with some method of constructing the one electron-potential function appropriate to the alloying species. Given this information, the electronic states of a random alloy can be calculated without further approximation save for the CPA itself. Thus, the KKR-CPA method focuses attention on the underlying one electron potential function $V(r)$ of the alloy. To date, $V(r)$ has been obtained by various ad hoc procedures, such as the Mattheiss prescription⁵ and the renormalised atom method⁶, together with possible slight adjustments of the potential to force agreement with some experimental results. In an alloy, this is a particularly unsatisfactory situation since the physical properties of the alloy are sensitive to the charge rearrangements which accompany alloying. Ideally, these charge rearrangements should be obtained ab initio. This has now been accomplished⁷ within the density functional approach of Hohnberg-Kohn-Sham (HKS)^{8,9}.

*Work sponsored by the Division of Materials Sciences U.S. Department of Energy, under contract W-7405-eng-26 with the Union Carbide Corporation. GMS gratefully acknowledges the support of a SERC Senior Visiting Fellowship at Daresbury Laboratory under CCP9.

Because the CPA is a single site theory the natural generalisation to alloys of the SCF-method for ordered solids is to make the single site average charge densities $\rho_{A(B)}$ (for the case of a binary AB alloy) self-consistent with the single-site average potential functions $v_{A(B)}$. Like the self-consistent band theory of ordered systems the SCF-KKR-CPA then consists of the following steps: (a) construction of initial $v_{A(B)}$ muffin tin potentials using some ad hoc method, (b) solution of the KKR-CPA equations throughout the occupied conduction band and calculation of the single site charge densities $\rho_{A(B)}$, (c) calculation of new $v_{A(B)}$ muffin tin potentials from the $\rho_{A(B)}$, (d) return to step b. Exit from the loop occurs when the difference between input charge densities (or potentials) for two consecutive iterations is less than some tolerance. In our SCF-KKR-CPA method the previously time consuming step (b) is facilitated by an accurate and rapid real space cluster method for solving the KKR-CPA equations⁷.

In fig.1 we show the densities of states obtained from our SCF-KKR-CPA calculations for three concentrations of the $\text{Ag}_c\text{Pd}_{1-c}$ alloy system. The local exchange correlation potential used was that of Hedin-Lundquist¹⁰ and the Ag and Pd atomic cores were frozen. The calculations were performed using a six nearest neighbour-shell cluster in the solution of the KKR-CPA equations. The densities of states shown are also those obtained using the cluster method. The fact that we have used the approximate cluster method makes no difference to the resulting self-consistent potentials. However, some of the fine structure in the densities of states of fig.1, at bottom of the Ag sub-band in the $\text{Ag}_{.8}\text{Pd}_{.2}$ alloy and at the top of the Pd-band for the $\text{Ag}_{.2}\text{Pd}_{.8}$ alloy, results from the fact that we used KKR-CPA solutions for the six-shell cluster to calculate the densities of states. In fig.2 we compare the SCF-densities of states with those obtained by Pindor et al³ on the basis of ad hoc potentials constructed using the Mattheiss prescription⁵. The SCF-KKR-CPA densities of states shown in fig.2 were those obtained after one final iteration using the time consuming Brillouin zone integration method of solving the KKR-CPA equations of Stocks et al. The differences between this curve and the corresponding curve in fig.1 reflect the errors introduced into the calculation of the density of states by using the cluster method.

For the $\text{Ag}_{.2}\text{Pd}_{.8}$ alloy of fig.2 the major effect of self-consistency is to move the low-energy Ag related peak closer to the Pd d-band complex and to increase the hybridisation between the Ag and Pd sub-bands. The shift in the position of the Ag d-band brings it into closer agreement with the results of the XPS measurements of Hufner et al^{3, 11}. For the nonself-consistent potentials, the center of the Ag sub-band is 5.9 eV below ϵ_F , this calculation gives 5.5 eV, experiment yields 5.4 eV. Small differences between the self-consistent and non-selfconsistent calculations exist for all concentrations, with experiment favouring the SCF calculations.

The methods which we have developed for performing these SCF-KKR-CPA calculations are not particularly time consuming on a scale set by present day band structure calculations on ordered systems having complex lattices. When are used in conjunction with modern vector processing computers such as the CRAY-1 at Daresbury we are able to perform SCF-KKR-CPA calculations at the cost of a few minutes of CPU per concentration.

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FIGURE CAPTIONS

Fig.1 Calculated densities of states for three $\text{Ag}_c\text{Pd}_{1-c}$ alloys using the SCF-KKR-CPA method detailed in the text.

Fig.2 Total and component densities of states for a $\text{Ag}_{0.2}\text{Pd}_{0.8}$ random alloy. Solid line: SCF-KKR-CPA. Dashed line: non-selfconsistent potentials of Pindor et al³. The upper frame: total density of states. Middle frame: density of states in Pd Wigner-Seitz cell. Lower frame: density of states in Ag Wigner-Seitz cell.

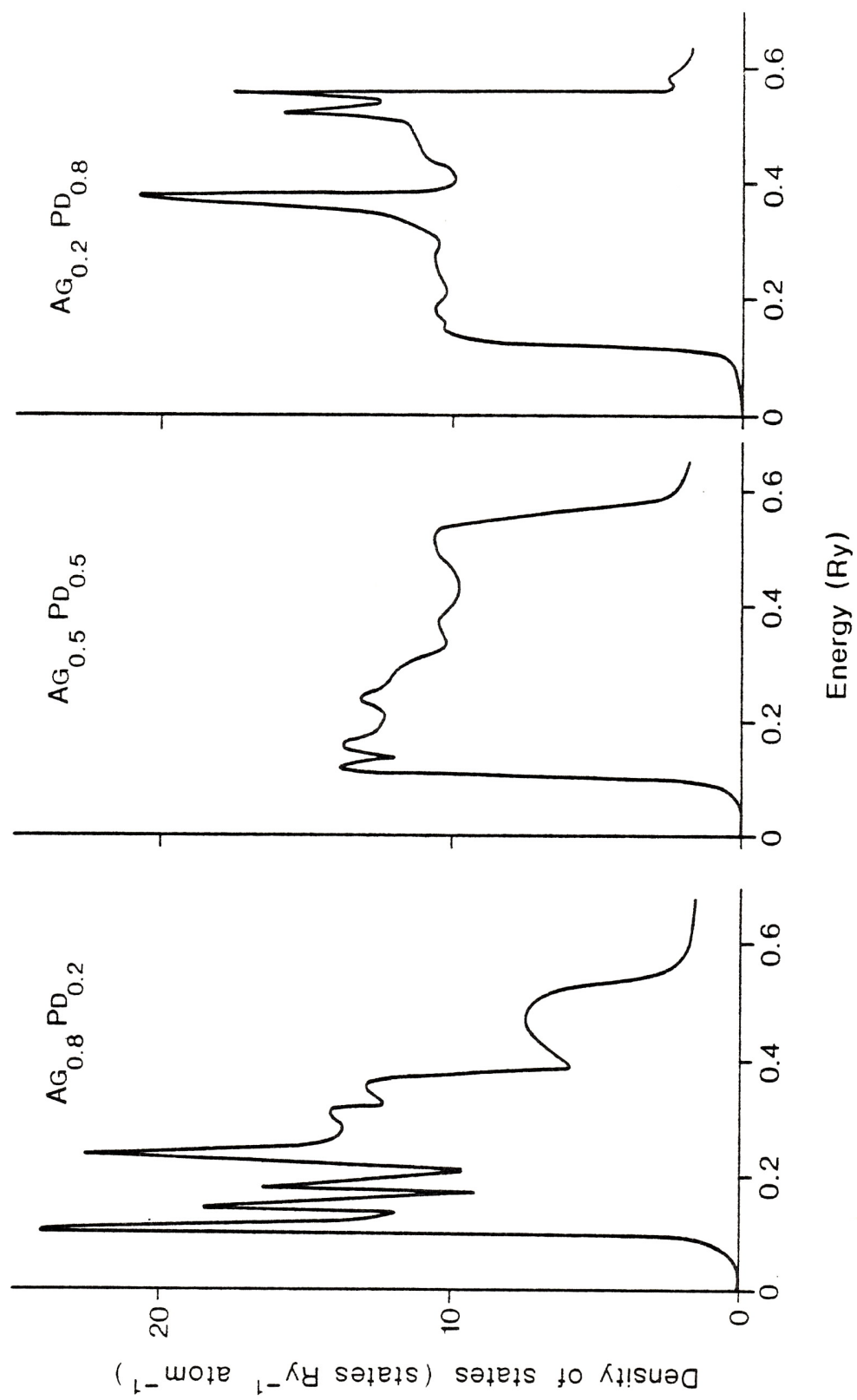


Fig.1

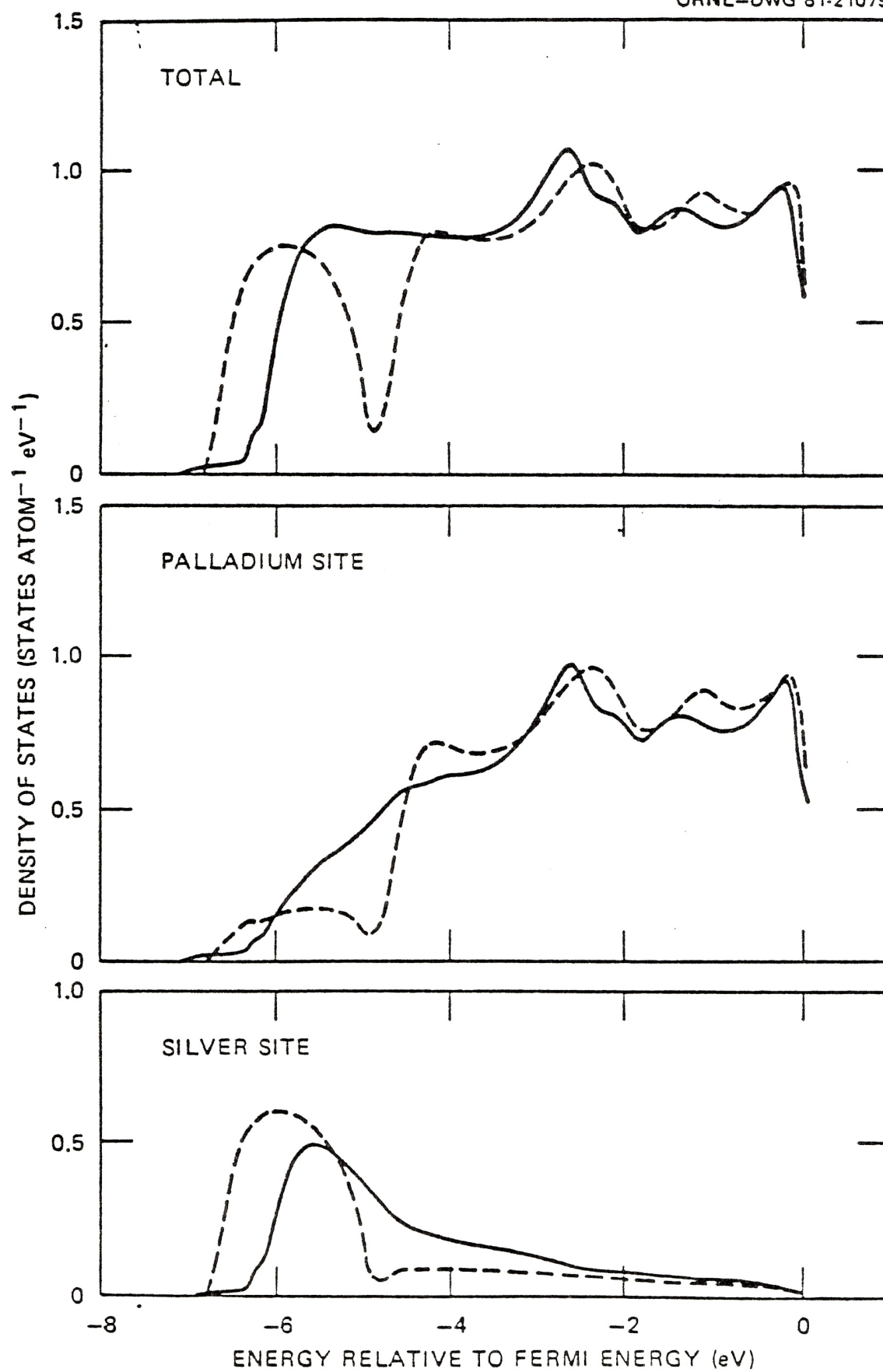


Fig. 2

ATOMIC-ORBITAL-BASED METHODS FOR COMPLEX SOLIDS

D.W. BULLETT

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(Abstract for Daresbury meeting on "Electronic Structure of Complex Solids",
24th November 1981.)

In this talk I will review five recent applications of atomic-orbital methods to the electronic structure of very complex systems:

1. Structure and bonding in crystalline boron and $B_{12}C_3$.
2. Variation of electronic properties with structure of the transition metal trichalcogenides.
3. Phase transitions on $W\{100\}$ and $Mo\{100\}$.
4. Adsorption of Cl on $Cu\{100\}$.
5. Surface states at alloy surfaces.

1. BORON

The first complete set of electronic structure calculations are reported for elemental boron in its α -rhombohedral (12 atoms per unit cell), β -rhombohedral (105 atoms) and suggested α -tetragonal (50 atoms) crystalline forms. The results show that a band picture provides an accurate description of the bonding in these solids. The α -rhombohedral structure is found to produce semiconducting properties, with an indirect gap of 1.7 eV. The ordering of bands can be qualitatively interpreted in terms of the internal molecular orbitals of a B_{12} icosahedron and the two-centre and three-centre external bonds linking neighbouring icosahedra. Replacement of the electron-deficient bonds by linear C_3 units gives the much stronger $B_{12}C_3$ structure, in which the calculated gap increases to a direct 3.8 eV. In the more complicated β -rhombohedral elemental structure, a forbidden gap ~ 2.7 eV occurs in the spectrum of electron states. Some degree of defect- or impurity-induced disorder seems essential to stabilise the structure, since the valence band of the 'ideal' structure can accommodate 320 electrons per unit cell, compared with the 315 available. In the suggested α -tetragonal modification of pure boron, the electron deficit would be so severe that this structure probably occurs only for compounds such as $B_{50}C_2$ and $B_{50}N_2$.

J. Phys. C (1981) to be published

2. TRANSITION-METAL TRICHALCOGENIDES

Electron band structure calculations reveal that ZrSe_3 is a semiconductor with $E_g \sim 1.5$ eV whereas NbSe_3 and TaSe_3 are both highly anisotropic metals. The Peierls transition in NbSe_3 is related to the presence of four quasi-one-dimensional free-electron-like bands crossing the Fermi energy. This feature does not exist in TaSe_3 , and the differences in properties are related to structural differences.

J. Phys. C (1979) 12, 277 and to be published

3. W{100} AND Mo{100} SURFACES

Here we compare the electron surface-state band structure of the (1×1) high-temperature phase and the $(\sqrt{2} \times \sqrt{2})R45^\circ$ W{100} reconstructed surface. The energy driving the low-temperature reconstruction appears to originate in the splitting of a partially occupied band largely confined to the surface layer.

4. ADSORPTION OF Cl ON Cu{100}

Calculations of the electronic structure of $\text{Cl}/\text{Cu}(001)$ are used to discriminate between contending adsorption sites from the electron distribution curves in normal photoemission previously reported. Adsorption above surface Cu atoms is ruled out. Either the four-fold-hollow site or a surface reconstruction would be consistent with the data; angle-resolved data for off-normal emission favour the four-fold-hollow site.

Solid State Commun. (1981) 38, 969

5. ATOMIC APPROXIMATION FOR ALLOYS AND ALLOY SURFACES

I will finish by making some remarks about the possible use of atomic-orbital-based methods to elucidate the surface electronic structure of random alloys.

Linearised augmented plane wave (LAPW) method for solids and solid surfaces

Greg A. Benesh

The traditional Augmented Plane Wave (APW) method is based on the muffin-tin (MT) approximation to the crystal potential. In the MT spheres the potential is taken to be spherically symmetric; while in the interstitial region the potential is constant. This model potential is used to define basis functions which are solutions of the Schrodinger equation appropriate to each region. Inside the α^{th} MT sphere, the solutions to the Schrodinger equation can be written as the product of a spherical harmonic and a radial function satisfying the equation

$$\left\{ -\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + \frac{\ell(\ell+1)}{r^2} + v_{\alpha}(r) - E' \right\} u_{\ell, \alpha} = 0 \quad (1)$$

When solving this equation for the free atom, two boundary conditions are imposed: regularity at the origin and vanishing magnitude at infinity. In the present case there is only the boundary condition at the origin to be imposed since the radial function is only defined within a MT sphere. Without a boundary condition on the MT sphere, the energy E' can take on any value. The APW functions are then defined as a linear combination of these solutions:

$$\phi_m^{\alpha}(\vec{k}, \vec{r}) = \sum_L A_{L, \alpha}^m(\vec{k}) u_{\ell, \alpha}(E', r) Y_L(\vec{r}) \quad (2)$$

In the interstitial region the potential is constant; we may rigidly shift the whole potential so that our zero of energy is defined as this interstitial constant. Solutions of the Schrodinger equation in this region are simply plane waves. These plane waves are the APW functions:

$$\phi_m^\alpha(\vec{k}, \vec{r}) = \left(\frac{1}{\Omega}\right)^{1/2} e^{i(\vec{k} + \vec{g}_m) \cdot \vec{r}} \quad (3)$$

where \vec{g}_m is a three-dimensional reciprocal lattice vector that refers the \vec{k} -vector to the first Brillouin zone.

In the usual form of the APW method, the basis functions are made continuous by matching across the MT spheres. This matching defines the $A_{L, \alpha}^m$ coefficients in Eq.(2). However the basis functions continue to have a discontinuous slope at the boundary of the two regions.

The crystal wavefunctions are then expanded as a linear combination of the APW's. A variational expression for the energy is then minimized with respect to the expansion coefficients, resulting in a set of secular equations. A simplification in the evaluation of the matrix elements can be made if we first consider the portion:

$$H_{mn}^{MT} - E(\vec{k})S_{mn}^{MT} = (E' - E)S_{mn}^{MT} \quad (4)$$

The practice has been to take the energy parameter E' equal to the energy eigenvalue E , thus simplifying the evaluation of the matrix elements and reducing the number of basis functions required. However, the secular equations become non-linear since the basis functions, and hence the matrix elements, now depend on the energy implicitly. In order to solve the problem the zeroes of the determinant must be found by re-evaluating for different energies. For even a moderately sized matrix this requires an order of magnitude more computation than does solving a linear set of equations.

Although the APW method has been extremely successful over the years, it does have a few disadvantages. The largest one is this computational problem of finding the zeroes of the determinant and then solving the equations. If the matrix elements were energy-independent then the whole process could be improved.

The Linearised Augmented Plane Wave (LAPW) method was developed to overcome the disadvantages of the standard APW method. Instead of using only radial wavefunctions inside the MT spheres, the basis set has been enlarged to include energy-derivative functions. The inclusion of these functions effectively eliminates the energy-dependence of the matrix elements since over some energy range we can approximate a radial wavefunction by the first two terms in a Taylor series expansion

$$U_{\ell}(E) = U_{\ell}(E') + (E - E') \dot{U}_{\ell}(E') \quad (5)$$

$$\text{where } \dot{U}_{\ell}(E') \equiv \left. \frac{\partial U_{\ell}}{\partial E} \right|_{E=E'}$$

The energy range over which this expansion is valid appears to be about 1 Rydberg for s and p bands and .2-.4 Rydbergs for d bands.

The LAPW basis functions inside the MT spheres are defined as a linear combination of both the regular and energy-derivative functions.

$$\psi_m^{\alpha}(\vec{k}, \vec{r}) = \sum_L \{ A_{L, \alpha}^m(\vec{k}) U_{\ell, \alpha}(E', r) + B_{L, \alpha}^m(\vec{k}) \dot{U}_{\ell, \alpha}(E', r) \} Y_L(\vec{r}) \quad (6)$$

The basis functions can now be matched both in value and first-derivative to the interstitial planewaves. The continuous slope of the LAPW's eliminates the asymptote problem - a minor disadvantage of the APW method.

The calculations that we have performed are self-consistent. This has been achieved by solving the secular equations at special \vec{k} -points, filling the bands by using Fermi-Dirac statistics, generating the corresponding charge density, and solving Poisson's equation for a new potential. The total Hamiltonian can be written as

$$H = H_{MT} + V_I + V_{NS} , \quad (7)$$

where H_{MT} represents the kinetic energy term plus the MT potential. V_I

and V_{NS} represent the interstitial and non-spherical potential corrections, respectively. Inclusion of only the first two terms on the right side of Eq.7 implies the so-called 'warped' muffin-tin potential. We have included not only these terms, but have also approximated V_{NS} . However, in evaluating the matrix elements of V_{NS} we have used the interstitial plane waves. This is reasonable because the plane waves match continuously and differentially on to the MT basis functions, so we expect them to be a good representation just inside the spheres where the non-spherical terms are the largest. We have thus extended the warping to just inside the MT spheres, thereby creating a 'corrugated' MT potential.

An interesting material that we have been looking at is the layered compound 1T-TiS₂. Over the years a tremendous amount of experimentation has taken place on this material and the isoelectronic compound TiSe₂. Current opinion, based largely on pressure studies of the Hall coefficient, favours a semimetallic picture for TiSe₂ and a semiconductor one for TiS₂. Our calculations and those of Temmerman, however, show conduction and valence band overlap in both materials. Our bandstructures compare quite well with angle-resolved photoemission experiments for both TiS₂ and TiSe₂. However, we have found a significant difference in the dependence of the bandstructures on pressure. Under 20 kbar of pressure the TiS₂ band overlap is unchanged to better than 0.01 eV, as is the shape of the conduction band. In contrast the TiSe₂ band overlap increases by over .2 eV, with a significant change in the shape of the bands. We think that this difference in the bandstructure might account for the difference in the pressure dependence of the Hall coefficient.

To summarise, the APW has been a very successful method and has been applied to a variety of interesting problems. However, there are a few disadvantages with it and the LAPW method was designed to overcome them. The LAPW method is extremely flexible, having been applied to bulk, surface, and now even molecular problems. TiS₂ may be a semimetal.

Linearised muffin-tin orbital (LMTO) method for complex solids

W.M. Temmerman (DL)

The linearized muffin-tin orbital band structure methods¹ enable us to perform band structure calculations at different levels of accuracy. We note the highly accurate LMTO calculations of Jones, Harris and Gunnarson² and the cruder LMTO-ASA calculations of such systems as the A-15 compounds³, chevre phases⁴.

The linearized band structure schemes combine the advantages of the bound state approach (LCAO) with the advantages of the partial wave methods (KKR,APW).

O.K. Andersen initiated the ϕ - $\dot{\phi}$ formalism: the expansion of the radial wavefunction of a single muffin-tin potential in the basis functions

ϕ and $\dot{\phi}$: $\phi(E,r) = \phi(r) + (E-E_V)\dot{\phi}(r) + \dots$ Therefore these basis functions can provide solutions of arbitrary accuracy for the muffin-tin potential model like the partial wave methods. Other linearized band structure methods include the ASW developed by A.R. Williams⁵ and the pivoted-multiple-scattering band theory of J.S. Faulkner⁶.

In this talk I quoted as examples the self-consistent LMTO-ASA band structure calculations of the layered compounds TiS_2 , TiSe_2 and their intercalates with Li⁷ and also the pyrites FeS_2 ⁸. For TiS_2 and TiSe_2 comparison with the more accurate LAPW band structure calculations⁹ is possible and we found agreement within 0.5eV. More importantly as in the LAPW calculations we obtain a semi-metal for TiS_2 with a band overlap of $\sim 0.7\text{eV}$.

We conclude that at the expense of this loss in accuracy we obtain very rapidly self-consistent potential functions for complicated structures. The performance of those calculations on the Cray 1S at DL was: for 6 atoms per unit cell, h.c.p. Brillouin zone, 105.k points in the $\frac{1}{12}$ of the Brillouin zone it takes 38 sec per iteration in the self-consistency cycle; for 12 atoms per unit cell, s.c. Brillouin zone, 55.k points in the $\frac{1}{24}$ of the Brillouin zone it takes 98 sec per iteration in the self-consistency cycle.

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Band Structure of the Pseudo-one-dimensional $M Mo_3X_3$
Transition-metal-compounds

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The compound $In_{1.2} Mo_6S_8$ has been found to exist with the Chevrel-phase structure and while attempting to make $In Mo_6Se_3$ the superconducting compound $In_{1.2} Mo_{15}Se_{19}$ was found¹. This differs from the Chevrel phase compounds in that as well as Mo_6Se_8 units there is now a second building block Mo_9Se_{11} . This unit may be regarded as being composed of two Mo_6 units fused along a common octahedron face. While trying to form a compound composed entirely of these Mo_9 clusters new compounds² containing equal numbers of Mo_6 and Mo_{12} clusters were obtained. The latter cluster arises from the linear fusion of three Mo_6 clusters. One can see that in principle this series may be continued to infinity and in fact several compounds³ $M Mo_3X_3$ have been reported where M is either Na, K, Rb, Cs, In or Tl and X is a chalcogen Se, S or Te. The isostructural iron compound $TlFe_3Te_3$, was found independently of the above mentioned development.

The crystal structure is hexagonal and is characterized by the presence of one dimensional chains running in the direction of the hexagonal c axis and separated by parallel chains of M atoms. There is a screw axis consisting of a translation $c/2$ along the c-axis followed by a rotation through 180° .

The intra-chain Mo-Mo bond lengths are very close to the intra-cluster bonds observed in other ternary Mo chalcogenides and also the nearest neighbour distance of Mo metal (2.72 \AA). The shortest Mo-Mo inter chain distance is greater than 6 \AA so that there is essentially no direct d-d overlap and electronic inter-chain coupling takes place through two X atoms, this weak coupling giving rise to the anisotropy in the physical properties⁵.

The only one of these compounds known to be superconducting TlMo_3Se_3 has a transition temperature of 3^0K . The ratio of the parallel to perpendicular critical magnetic field is about 26. The observed normal state resistivity ratio is approximately $1000 \sim 26^2$. This is the only compound to have been studied experimentally in any detail⁵.

We have calculated the bandstructures of these compounds using the LMT0-ASA method⁶ and the Mattheiss description for the one-electron potential. The bandstructure of TlMo_3Se_3 is shown in Fig. 2 for k along the c-direction. The existence of a screw axis allows us to fold the bands out into a double zone corresponding to a TlMo_3Se_3 unit cell. There is a three-fold axis through the centre of each column which gives rise to doubly (heavy lines) and singly (light lines) degenerate representations. If metal-ligand hybridization is neglected then the Mo d states form a complex $.5 \text{ Ryd}$ wide which overlaps the $.3 \text{ Ryd}$ wide Se p bands to a large extent. The separation of the band centres is 0.23 Ryd . The effect of including the hybridization is to open up a 100 mRyd wide gap at -0.7 Ryd which is crossed by a singly degenerate broadly dispersed d band which we call a Helix band because of its xy character (see Fig.1). The bands below the gap have mixed metal d-ligand p character. In addition there is a singly degenerate band arising from the Tl 6s state. Above the gap the bands have mostly metal d character. The lowest lying of these bands is doubly degenerate and has a very small occupancy. It has equal amounts of $3z^2-r^2$ and x^2-y^2 character and we call it the octahedron band

because it is one of the bands derived from directed orbitals pointing towards the centre of the Mo octahedra making up the chain.

The calculations show that the Fermi surface comprises two sheets at $\pm k_F$ perpendicular to the c axis arising from the Helix band and two small concentric ellipsoids at A arising from the octahedron $O_{t_{1u}}$ band. This agrees with the magnetoresistance experiments which show that there may be open orbits perpendicular to the c axis but not along the c axis.

The sheets have a slight wobble proportional to the dispersion in the directions perpendicular to the chain. Near $k_x = \pm \pi/c$ they may be parametrized by the first few terms of its Fourier series. This expression represents the computed bands very well and allows an analytical evaluation of the mass tensor and hence of the anisotropy parameter ϵ for the sheet. We find values of ϵ for the sheet between 18 and 50. The reason for this spread in values comes from the uncertainty in the dispersion perpendicular to the chains which is about 1 mRyd. The density of states from the sheet is about 0.6 states/Ry·Mo.at.spin. Even allowing for phonon enhancement this value is too low in comparison with the value of 3.0 derived from the specific heat measurements.

Turning our attention now to the ellipsoidal pockets we find that their volume is very sensitive to our choice of sphere sizes in the ASA. The helix band at π/c and the octahedron band at A have a maximum overlap of 10 mRyd for space filling spheres. This then sets a maximum occupancy of the ellipsoid at 0.1 electron. The ellipsoid then dominates the anisotropy which is reduced from 18 to 7 and also the density of states which is 3.2 states/Ry·Mo.at.spin giving a total of 3.7. By choosing slightly smaller spheres we can obtain agreement for both anisotropy and density of states.

There is another reason for believing that there are two bands at the Fermi level. If there were no overlap the structure would be unstable against any distortion which would destroy the 2-fold screw axis and open up a gap at π/c . The ellipsoidal pockets should be experimentally verifiable.

The band structures computed for the remaining Tl and In selenides and tellurides are almost identical to that of TlMo_3Se_3 and show no clear trends in the overlaps. The reason why none of the other chain compounds has been found to be superconducting is either that the overlap is so small that the density of states is very low or that a Peierls distortion has taken place. So far no such structural phase transition has been observed but the atomic rearrangement necessary to create a gap could be very subtle such as a relative twist of the alternating Se-triangles. If more than 13 electrons were present the Fermi level would move up into a high density-of-states region and this would destabilize the crystal structure. If less than 13 electrons were present the columns would break up as the result of a Peierls distortion and phases containing chain fragments like bioctahedra, trioctahedra etc. would be more stable. Such phases have indeed been found and this may explain why TlMo_3Se_3 is found to be stoichiometric. If the ellipsoid is the reason for the superconductivity and stability of TlMo_3Se_3 then it should be possible to control this by doping or applying stress.

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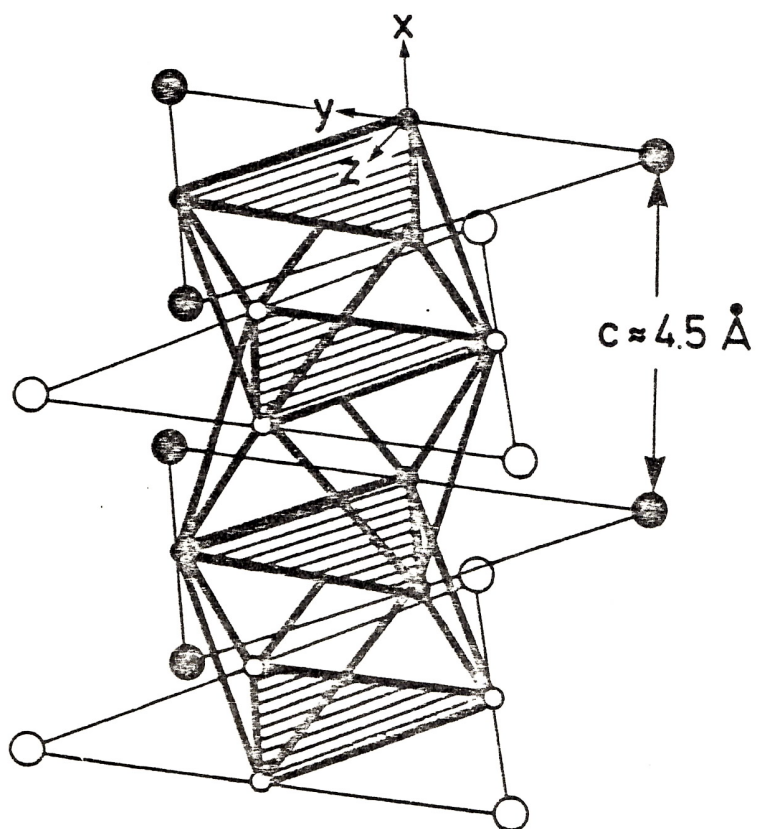
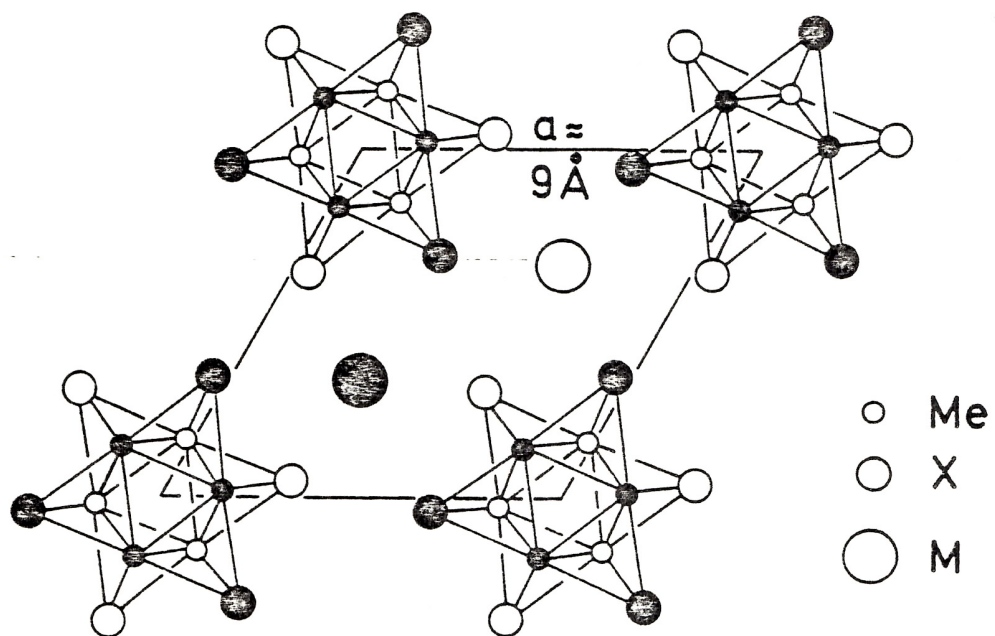


Fig 1

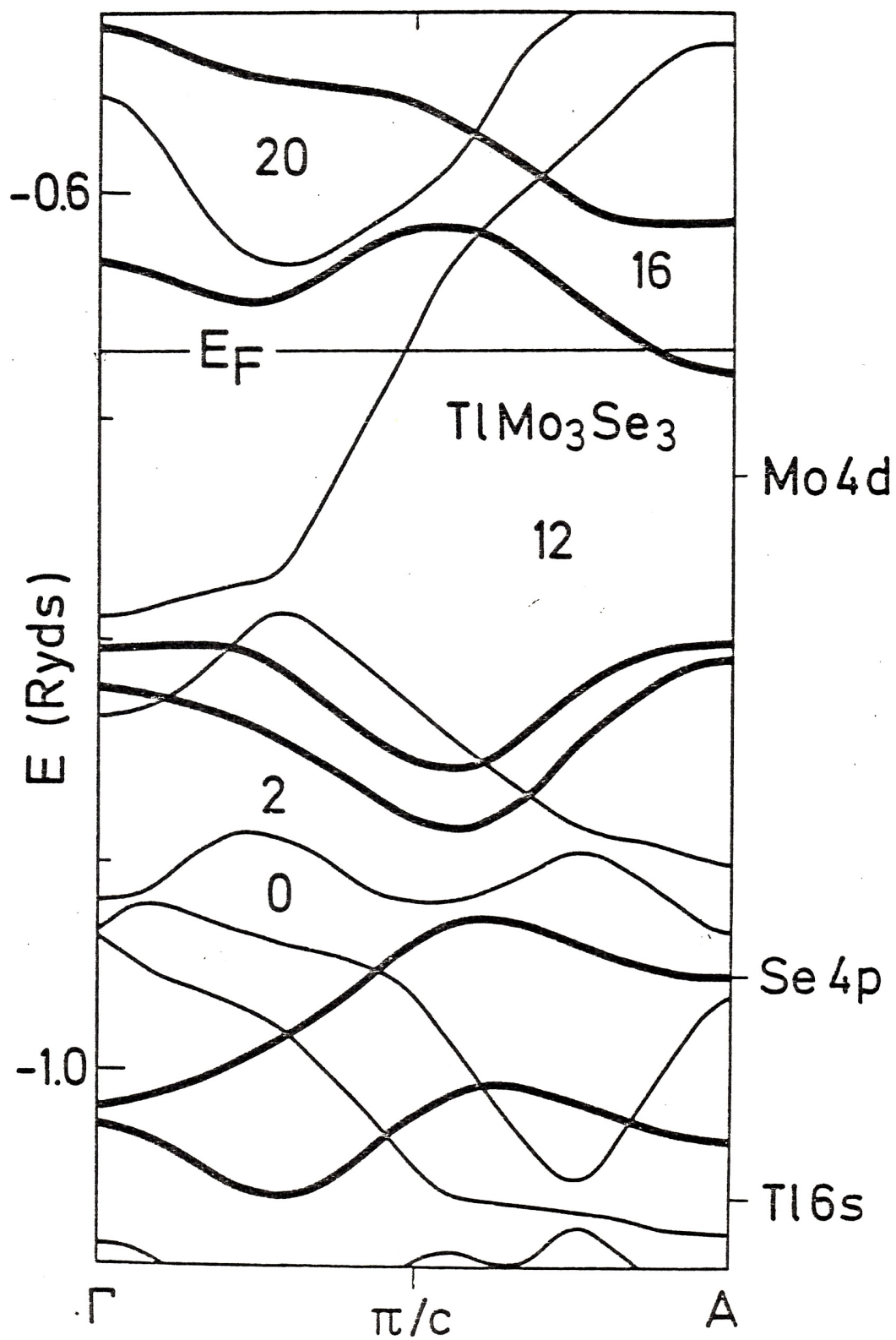


Fig.2

EMBEDDING CLUSTERS OF ATOMS AND SURFACE LAYERS

J.E. Inglesfield

SERC Daresbury Laboratory, Daresbury

One of the most common methods of calculating the electronic structure of impurities in solids, or surfaces, is to consider a finite cluster of atoms, or a slab consisting of a few layers; although this is probably satisfactory for calculating very local properties like charge density it is less good for calculating densities of states because of surface states associated with the spurious surface of the cluster. To deal with this I have developed a new embedding method¹ in which a surface potential is added to the Hamiltonian for the cluster, or slab, which ensures that the wavefunctions match correctly onto the wavefunctions of the substrate. This surface potential can be calculated once and for all from the Green function for the perfect substrate. The advantage of this method is its flexibility, and any basis set can be used in the cluster - there are no muffin-tin restrictions, and atomic relaxations can be immediately included. As a first non-trivial application of the method I have used it to calculate the density of states and charge density of a H interstitial in Cu, going to self-consistency not only in the impurity cell but also in the neighbouring Cu cells². There is ^c/H-Cu bonding level near the bottom of the Cu conduction band, but I also find a large downward shift in the energy of the neighbouring Cu d-levels due to interacting with the proton. The embedding technique is now being applied also to surface problems, using LAPW's in the surface layer with an embedding potential found for the substrate using the layer doubling method.

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CURRENT STATUS OF THE RECURSION METHOD

Roger Haydock, Cavendish Laboratory, Madingley Road,
Cambridge CB3 0HE UK

The recursion method (Haydock 1980) is a way of approximating elements of the greenian (resolvent) of large (or even infinite) matrices. It is related to the Lanczos method (Parlett 1980) in that both methods use an algorithm, for tridiagonalizing a matrix having real eigenvalues, which arises in the solution of the classical moment problem.

Since 1972, the recursion method has been applied to a wide variety of calculations of electronic structures which require large basis sets. These include complicated crystals such as the Laves phases of transition metal compounds, random network models of amorphous semiconductors and metallic glasses, strong ferromagnets above the Curie point, localization in the Anderson model, and surfaces of transition metals. The hamiltonians for these systems have been expressed as tight-binding models, but the method is applicable to gaussian bases, nearly free electron models (in a momentum representation), and hybrid models. There has also been some work on self-consistency. Results are usually presented as local (projected) densities of states, although k-dependent spectral functions have also been used. When the algorithm is applied as the Lanczos method, accurate eigenvalues and eigenvectors are produced.

In practice, computations may be carried out on square matrices whose dimension (number of rows) is up to half the number of storage locations, provided the matrix can be stored in a condensed form. For matrices of large dimension, N (greater than 100), the time required is proportional to N^2 , faster than standard methods such as Householder's which takes a time proportional to N^3 . In addition much information can be obtained from only a partial tridiagonalization. The results (bounds on indefinite integrals of local elements of the resolvent, eigenvalues and eigenvectors) are accurate to about one rounding error.

Recently, the methods for estimating local densities of states (LDOS) of infinite systems have been improved (Nex 1978). Rigorous bounds can be placed on the indefinite integral of the LDOS and the best estimate of the LDOS is obtained by differentiation of the mean of these bounds. This replaces previous methods where the infinite tridiagonal matrix was approximated by constant elements for those not calculated.

The recursion programs have been modified so as to take advantage of pipelining and are available on the Cray at Daresbury. In addition to the faster cycle time of the Cray, if basis elements are blocked in groups of 64 (implemented as number of orbitals per atomic site in a tight-binding model), the speed is increased by a large factor over the same calculation without blocking. Experiments show the factor to be 2 or 3 for blocks of 5 orbitals. Does this go up to a factor of about 60 for blocks of 64 orbitals? This has not yet been tried.

Documentation of the recursion library is available from C.M.M. Nex, Cavendish Laboratory. D.G. Pettifor, Dept. of Mathematics, Imperial College, coordinates the recursion project under CCP9.

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CCP9 Project 1: Cluster Calculations

Spokesman: J.E. Inglesfield

Collaborators: G. Benesh (Cambridge), Neil Cade (QMC), Paul Durham (DL), Balazs Gyorffy (Bristol), John Inglesfield (DL), Roy Jacobs (Imperial), Peter Lee (Lancaster), N. Miller (Lancaster), John Pendry (Imperial), Delano Saldin (Imperial), Malcolm Stocks (DL), Walter Temmerman (DL), Denis Weaire (University College, Dublin).

Programs currently available: These include a KKR scattering wave cluster program used by M. Stocks in CPA calculations, scattering programs used by P. Durham and J.B. Pendry in XANES and cluster LEED calculations and liquid theory. All these use a muffin tin form of potential. Tight-binding programs using the recursion method are available at Cambridge, though these are best suited for much larger clusters than are envisaged in this project. J.E. Inglesfield has developed a self-consistent LMTO cluster program to deal with a tetrahedral cluster of atoms around an impurity for embedding into a host metal. An LMTO program has also been brought by W. Temmerman from Stuttgart for self-consistent calculations in crystals, and this should be readily adaptable to give a self-consistent LMTO cluster program.

Programs being developed: None of the existing programs can deal with an arbitrary cluster, with an arbitrary potential self-consistency, and it would seem desirable to develop programs which can actually do this. An embedded self-consistent KKR cluster program is currently being developed by G.M. Stocks, working within the muffin tin approximation. J.E. Inglesfield is developing a general self-consistent LMTO cluster program.

Applications of cluster programs:

- (i) KKR cluster programs have been used by the Bristol group to study the properties of metallic glasses, at the moment calculating the density of states non-self-consistently.
- (ii) Impurities can be studied using cluster programs, preferably embedded, and Inglesfield has studied H-interstitial in metal.

Stocks and Temmerman are also working on impurities in metals, and Lee and Miller are starting work on impurities in semiconductors.

(iii) XANES and EXAFS calculations use cluster techniques (Durham and Pendry), and this is also being applied to LEED by Pendry, using the fact that the electron has a relatively short mean-free-path, and so the scattering by a cluster of atoms at the surface can be considered.

(iv) Clusters can be used to find the self-consistent field potential for use in KKR-CPA calculations - this technique is much easier than the usual k -space summation.

(v) Application of clusters to liquids by Pendry.

Role of CCP9: Perhaps the most useful role to begin with would be to encourage collaboration in the development of better cluster programs, which would then be generally available. J.E. Inglesfield would be grateful for collaboration in developing the LMTO cluster programs.

Further Development of the Korringa-Kohn-Rostoker-Coherent-Potential Approximation (KKR-CPA) method for studying the electronic structure of random alloys.

Collaborators: Dr. G.M. Stocks, Dr. W.M. Temmerman (SERC Daresbury, Dr. J. Staunton, Dr. B.L. Gyorffy (University of Bristol), Dr. A.J. Pindor (University of Cambridge).

As in the band theory of pure metals a time comes when one must consider calculating response functions in the theory of electronic structure of random alloys. The successes of KKR-CPA for calculating one particle properties suggest that it is a sound first principles basis to build on. This project aims to develop the necessary codes for the Brillouin zone integration which is the central part of calculating any susceptibility-like quantity. The first applications we shall have in mind are: electronic transport, concentration fluctuations and magnetic susceptibilities.

Spokesman: Dr. B.L. Gyorffy

CCP9 Project No 3: 'LMTO package'

Spokesperson: W. Temmerman

Collaborators: D. Glotzel, G.M. Stocks, J.E. Inglesfield, J.S. Faulkner

The aims of this project are to make the LMTO package more readily available to the user's community. I therefore plan to document this program as soon as possible.

This program linearizes at $\epsilon = V_{\text{mTZ}}$ only^{1,2} and we want to be able to improve on the accuracy in a systematic way through the implementation of pivoted-multiple-scattering^{3,4}. This will enable us to linearize or quadratesize at $\epsilon \neq V_{\text{mTZ}}$. Moreover we want to consider how to implement band theory with the PMS for general potential functions.

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CCP9 Project No 4: 'Relativistic and self-consistent KKR'

Spokesperson: Walter Temmerman

Collaborators: P. Weinberger, R. Podloucky, G.M. Stocks,
J. Staunton, B.L. Gyorffy

We obtained at DL a relativistic and self-consistent KKR program from Peter Weinberger. This program has now to be made up to date and optimized for use on the Cray.

In more detail we want to generalize this program to complicated structures. We also want to improve on the energy eigenvalues, search and the normalization of the wavefunction. To perform the Brillouin zone integral this program uses the special k point method, we feel that this should be replaced by the tetrahedron method.

Angular Correlation of (Positron) Annihilation Radiation (ACAR)

Collaborators: Dr. R. West and Mr. J. Kaiser (University of East Anglia), Dr. Z. Szotek, Dr. B.L. Gyorffy (University of Bristol).

The aim of the project: is to develop a comprehensive set of programs for the interpretation of 2d ACAR measurements on pure metals, intermetallic compounds and random metallic alloys. The calculations will be based on an effective independent particule picture and the KKR and KKR-CPA methods for solving the relevant Schrödinger equations. The electrons and the positron will be treated on equal footing and the end result will be the 2γ momentum distribution function $N_{2\gamma}(\vec{p})$ and its integrals over various portions of the Brillouin zone. The purpose of comparing theory and experiment will be to obtain information, not available from any other source, about the momentum distribution of conduction electrons.

Spokesman: Dr. B.L. Gyorffy

CCP9: The Recursion Project.

(c.f. R. Haydock's article in this issue of $\psi_{\underline{k}}$).

The recursion project will optimize the Cambridge recursion programme for use on the Cray machine. With the increased store and speed available it will study in detail the convergence properties of the real space Green's functions and related integrated quantities such as the non-local susceptibilities, and it will assess the best procedure for representing an infinite system with knowledge from only a finite number of levels. The programme will be tested for applicability in fields of research such as magnetism and non-local susceptibilities, force constants and lattice dynamics, and general questions of structural stability that arise, for example, in the treatment of dislocation cores and crack tips.

Collaborators: Co-ordinator: D. Pettifor: Mathematics Department, Imperial College.

C. Nex, E. Haines:	Cambridge.
D. Weaire:	Dublin.
C. Sayers:	Harwell.
R. Jacobs, R. Podloucky:	Imperial College.
W. Young:	Queen Mary College.

CCP9 Project No.7: Self-consistent LAPW

Spokesman: V. Heine

Collaborators: J.E. Inglesfield (DL), N. Cade (QMC), G. Benesh, A. Woolley, R. Godby (Cambridge).

G. Benesh brought a self-consistent LAPW programme to Cambridge in 1980. At first designed for calculations on thin slabs, it has now been extended to bulk bandstructures. He and J. Inglesfield are adding the capability to embed a slab onto the bulk. It is hoped that by the time Benesh returns to the USA in summer 1982, there will be sufficient familiarity with the APW programme by enough people to keep it operational in Britain.

Projects currently under way are as follows:

1. Transition metal surfaces: W(001) and Fe(001) (G. Benesh).
R. Haydock and G. Benesh are thinking about core shifts and d-sp calculations.
2. Layer compounds (TiS_2 and TiSe_2), leading toward intercalated compounds (G. Benesh and A. Woolley).
3. Embedding a slab onto the bulk (J.E. Inglesfield and G. Benesh).
4. Polymeric solids (N. Cade at QMC).
5. Adsorbates on transition metal surfaces: O in Ni(001) which Rex Godby is starting to do.
6. Forces on atoms and equilibrium atomic positions at an interface under shear. (Planned by R. Godby after Project 5).

Experimentalists are interested in comparing angle-resolved photo-emission spectra with calculated bandstructures. The LAPW bands seem to compare quite well both with bulk and surface bands. R. Willis is currently studying Fe(001) and both he and Dave King at Liverpool have been looking at W(001) with and without hydrogen. The calculations on TiS_2 have demonstrated some reason to reinterpret both angular resolved photo-emission measurements and pressure-dependent Hall coefficients: this relates to the experimental work off A. Yoffe's group in the Cavendish.

Inelastic neutron scattering

Two new neutron sources will become available in the near future. They are the new Harwell Linac (1982) and the Spallation neutron source (SNS) at the Rutherford Laboratory (1985). The Linac will make it possible to do inelastic scattering experiments involving higher energy transfers than are currently possible (~ 0.15 eV) at, for instance, I.L.L. The SNS will similarly allow a higher energy range to be probed, but with a beam of intensity two orders of magnitude greater than the Linac.

The inelastic scattering experiments envisaged involve energy transfers in the range ~ 0.2 eV to several eV - i.e. electronic transitions. An early experiment on the Linac will be on spin waves in the itinerant system nickel. Of particular interest is the optical mode and also the broadening due to interaction with single particle states (for background, see Mook and Tocchetti Phys. Rev. Lett. 43, 2029, 1979 and Cooke et al Phys. Rev. B21, 4118, 1980). With the SNS it should be possible to probe the single particle states themselves. Because neutron induced transitions are from occupied to unoccupied electronic states, there is the potential for gaining information about unoccupied states from the experiments, thus complementing data about occupied states already obtainable from photoemission measurements. New insight into the behaviour of itinerant magnetic systems and their alloys with each other and with non-magnetic systems is thus anticipated. A related experiment is the use of the neutrons to excite electrons across the band gap of a semiconductor. In principle it should be possible to extract information about the conduction band from the experimental data (a calculation of the cross sections to be expected from such an experiment has already been made by J.F. Cooke and J.A. Blackman - to be published - preprints are available from me).

There is a need to pursue the feasibility studies (such as the semiconductor one referred to above). It is also important to provide theoretical and computational support from the time of the first Linac experiments. I plan to have discussions with Stephen Lovesey (RAL) and Bill Mitchell (Oxford), who is directing instrumental developments, from which we hope to get the project under way. It is anticipated that John Cooke will be involved in the nickel studies. The KKR-CPA group (Gyorrfy, Stocks, Temmerman) has expressed interest in any alloy work.

The names of several people (apart from those already referred to) who would have some interest in the project have been mentioned to me. They are D.M. Edwards, R.J. Elliott, C.G. Windsor, E.P. Wohlfarth, W.H. Young. Doubtless there are omissions which I will be happy to rectify.

(J.A. Blackman)

This project aims broadly to develop programmes for the magnetic χ_m and dielectric χ_e susceptibilities for the paramagnetic, ferromagnetic and antiferromagnetic states of transition metals with various lattice structures. Initially the single particle energies and wavefunctions required as inputs may be taken to be those already developed for para- and ferromagnetic by O. K. Andersen and for antiferromagnets by N. A. Cade within the ASA LMT0 method in the local spin density (LSD) approximation. The Brillouin zone integration technique to be used may be the tetrahedron method with linear interpolation.

Obviously there is a whole host of outputs emanating from such a programme. The following are some suggestions as to how the outputs may be used and the sort of phenomena to which they may relate.

- (1) The static values of the unenhanced susceptibilities $\chi_m^\perp(q,0)$ together with an appropriate effective (Hubbard or Stoner like) electron-hole interaction calculated within the LSD formalism can provide stability criteria for ground states corresponding to various spin structures.
- (2) Evaluation of $\chi_m^\perp(q,\omega)$ within the random phase approximation (say) leads to the dispersion relation for the elementary excitations (spin waves). Inclusion of actual band structures with several bands will lead to a range of elementary excitations originating from interference between various orbitals. These and other higher energy excitations will be within range of experiments to be done with the exciting forthcoming spallation source.
- (3) Evaluation of both $\chi_m^\perp(q,\omega)$ and $\chi_m^\parallel(q,\omega)$ will lead to a complete determination of the neutron scattering cross-

section for all q and ω . In particular, by using the full band structure and its wavefunctions, the measured intensities can be computed.

- (4) To determine the atomic forces and phonons, the dynamical matrix $D^{ij}(q)$ is required. This involves evaluation of the dielectric susceptibility χ_e . One can examine the effects of both the long range Coulomb as well as the other short range (including the exchange-correlation) forces.
- (5) Through the inclusion of exchange enhancement in the magnetic ground states, one can study magneto-elastic effects. The various mechanisms for phonon softenings can also be investigated with particular reference to the band structures.
- (6) By evaluating the full dielectric response function matrix $\chi_e(q+G, q+G')$ (G, G' , are reciprocal lattice vectors), one can investigate the lattice dependent properties of the atomic forces. The various elastic constants may be evaluated and compared with those obtained by other methods.

I am sure that I have only just touched on the application of the above programmes. I have also been very subjective in the choice of inputs and computational techniques. I wish to emphasise that the above outline of this project is very preliminary and I would welcome any suggestions, comments, constructive criticisms, etc.

$\chi(q, \omega)$ Spokesman

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Elementary Excitations in Disordered Solids

D. Weaire.,

Physics Department, University College, Dublin.

A NATO Advanced Institute on Elementary Excitations in Disordered Solids took place at Michigan State University in August 1981. Many threads of current research in this area were drawn together at the meeting, and a personal account of its progress may be of interest to those involved in CCP 9.

"Elementary excitations" includes electronic states, vibrational spectra, and spin waves. "Disordered solids" include alloys, amorphous metals and semiconductors and (paradoxically) liquid metals. The relevant theoretical methods include selfconsistent theories of the CPA type, other types of cluster calculations (e.g. "cluster-Bethe"), the equation -of-motion method, the recursion method and closely related methods based on moments.

From one point of view, all of these techniques are means of avoiding the diagonalisation of very large matrices, which would yield answers to most physical questions by simply determining the properties of large samples in a direct manner. It is a pity, therefore, that few of those involved have any real "feel" for the recent progress of matrix methods, the comparative advantages of different library routines, etc. There should in future be a better interchange between computational physicists and specialists in numerical analysis.

Theories of the CPA type came under fire for being (a) full of awkward mathematical subtleties (b) requiring much more computing than it might appear. A stout defence against point (a) was made by Leath and Kaplan, who explained that recent progress in understanding, due to Mills and collaborators, had resolved many of the technical difficulties encountered in extending CPA to clusters. As for point (b), CPA enthusiasts maintained that their methods offer greater "insight" than rival (quicker) methods. Indeed,

Leath claimed the status of a "theory" for CPA, which he denied to the equation-of-motion and recursion techniques.

This may be so, but it seems clear that the experimentalist who wishes to test a particular model Hamiltonian in the interpretation of a particular experiment, without introducing theoretical complications, would do well to opt for the latter techniques, whenever they are applicable. The equation-of-motion method has proved particularly fruitful for spin waves (Buyers, Cowley), for which it has proved possible to study samples of up to 16,000 degrees of freedom. One drawback of the equation-of-motion and recursion methods is that they owe much of their efficiency to the short range of the interactions in the system to which they have been applied. Some thought needs to be given to the inclusion of weak interactions of longer range.

The proceedings of this institute should be a very useful guide to a subject which until now lies scattered in the literature, and will be published in the near future.

NATO ADVANCED STUDY INSTITUTE

UNIVERSITY OF GENT, BELGIUM

JULY 12 - 23, 1982

THE ELECTRONIC STRUCTURE OF COMPLEX SYSTEMS

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A.J. FREEMAN, NORTHWESTERN UNIVERSITY, EVANSTON, U.S.A.
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A.R. WILLIAMS, I.B.M., YORKTOWN HEIGHTS, U.S.A.
J. WILSON, UNIVERSITY OF BRISTOL, BRISTOL, U.K.

*ADVISORY COMMITTEE : Collaborative computational project on bandtheory
represented by B.L. Gyorffy, V. Heine and J.B. Pendry*

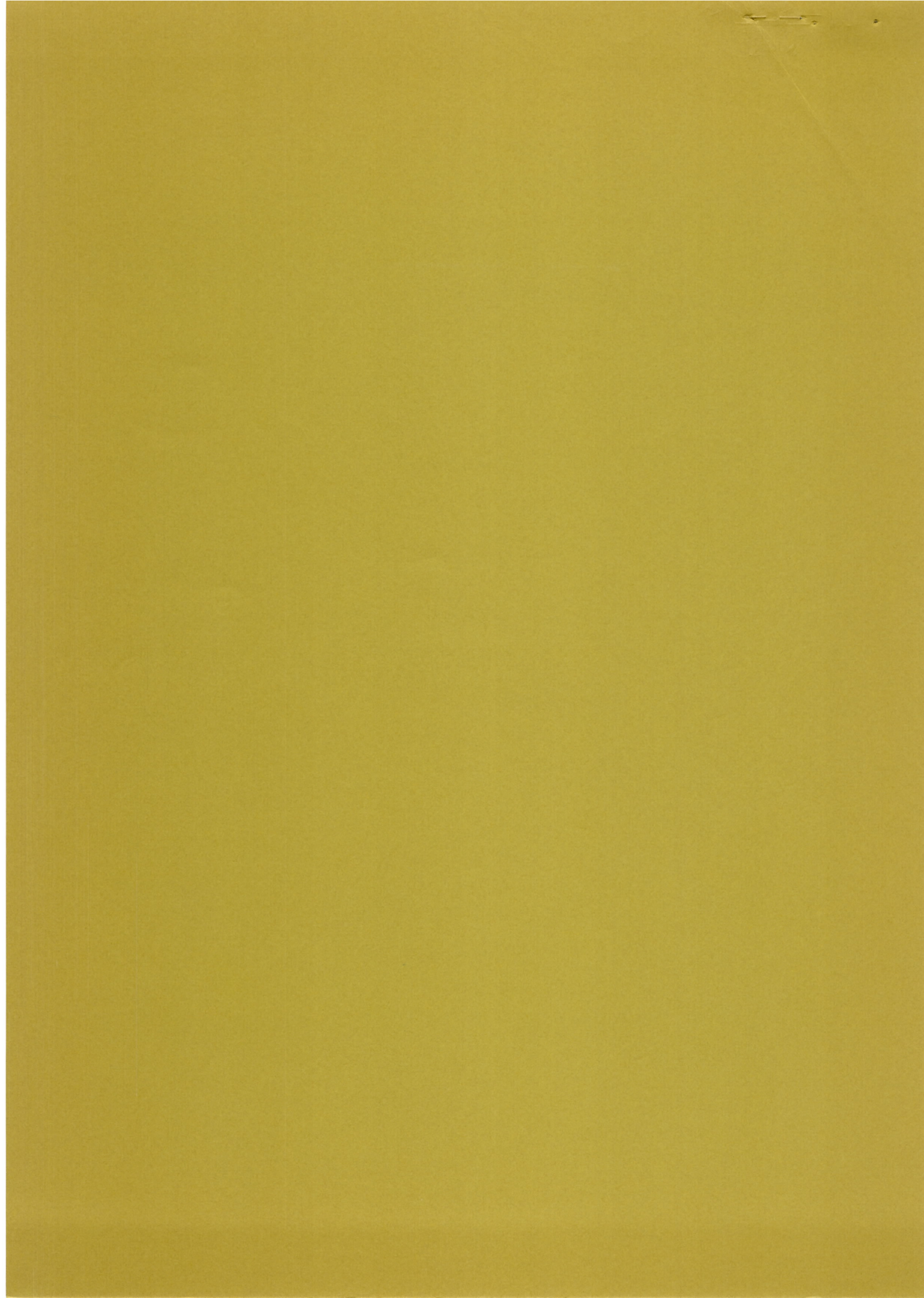
INFORMATION

P. PHARISEAU

Seminarie voor Theoretische Vaste Stof- en Lage Energie Kernfysica
Krijgslaan 281, Gebouw S9
B-9000 GENT (BELGIUM)

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NATO ADVANCED STUDY INSTITUTE
THE ELECTRONIC STRUCTURE OF COMPLEX SYSTEMS
GENT (BELGIUM) JULY 12-23, 1982

GENERAL INFORMATION

1. Purpose of the Institute

First principles electronic structure calculations are playing an increasing role in solid state physics. Theories of the solid state often rest on a series of assumptions which make the equations manageable. It is only through detailed computational studies that we are discovering which model is appropriate for a given material. The lectures at this summerschool will deal with the methods, the models and the results of first principles computations of the electronic properties of solids. The methods may be ab initio computations on simple materials or more parameterised ones for complex situations. One of the aims of this study institute would be to disseminate the present knowledge of bandstructure methods to solid state physicists.

2. Organizing Committee

Director : Prof. Dr. P. Phariseau, University of Gent, Gent, Belgium
Co-Director : Dr. W.M. Temmerman, SERC, Daresbury, U.K.

3. Content of the course

Prof. O.K. Andersen, M.P.I.F., Stuttgart, Fed. Rep. Germany :
Linear methods in bandtheory (5 lectures)

Dr. P.J. Durham, S.E.R.C., Daresbury, U.K. :
Spectroscopic studies of ordered and disordered metals (3 lectures)

Prof. A.J. Freeman, Northwestern University, Evanston, U.S.A. :
The bandmodel for d and f metals (5 lectures)

Dr. M. Gupta, Université Paris-Sud, Orsay, France :
Electronic Structure of metal hydrides (3 lectures)

Dr. B.L. Gyorffy, University of Bristol, Bristol, U.K. :
Spin polarized bandtheory with non-aligned spins (4 lectures)

Dr. J. Harris, K.F.A. Jülich, Jülich, Fed. Rep. Germany :
Density Functional Calculations for molecules (3 lectures)

Dr. G.M. Stocks, O.R.N.L., Oak Ridge, U.S.A. :

Electronic Structure of random alloys and impurities (5 lectures)

Dr. U. Von Barth, University of Lund, Lund, Sweden :

The density functional theory for solids (5 lectures)

Dr. W. Weber, K.F.Z. Karlsruhe, Karlsruhe, Fed. Rep. Germany :

First principles lattice dynamics (4 lectures)

Dr. A.R. Williams, I.B.M., Yorktown Heights, U.S.A. :

First principles energetics (5 lectures)

Dr. J. Wilson, University of Bristol, Bristol, U.K. :

Long-range order in d and f metal components (4 lectures)

4. Publication

The edited version of this course will be published in the NATO-ASI Series by Plenum Press.

5. Advisory Committee

The Collaborative Computational Project on bandtheory represented by Dr. B.L. Gyorffy (University of Bristol, Bristol, U.K.), Prof. V. Heine (University of Cambridge, Cambridge, U.K.) and Prof. J.B. Pendry (Imperial College, London, U.K.).

6. Attendance

This course is intended for young solid state physicists. The number of participants will be limited to 66. For graduate students a letter of recommendation from their research supervisor is required.

7. Application

All applications should be made on the enclosed form and returned not later than May 15, 1982. Successful applicants will be notified by June 1, 1982.

8. Accommodation

Housing for the participants will be arranged at the university residences. Accompanying dependants are welcome, providing they are willing to stay in single rooms at their own expense.

A contribution of 8,000 BFrs. towards the costs (including housing, meals, insurance, lecture notes, sightseeing and other social activities) for the entire period is required per participant.

9. Fellowships

For a limited number of accepted students, unable to obtain a travel grant from their own sources, a fellowship covering partially the travel expenses can be made available on request.

NATO Advanced Study Institute on
"The Electronic Structure of Complex Systems"
July 12 - 23, 1982
Rijksuniversiteit Gent, Belgium

APPLICATION FORM
(please type or print)

1. Name
2. First name(s)
3. Institution + address
4. Mailing address (if different from item 3)
5. Place and date of birth
6. Nationality
7. Sex : Male ☐ Female ☐
8. Academic Qualifications
9. Present professional activity
10. List of publications (or letter of recommendation)
11. If a travel grant is needed, indicate amount and justification and have this signed by the head of departments. Only a limited number of grants partially carrying travel is available.

Applicant's Head of Department to sign here :

12. The participant will be accompanied by persons

Place and Date :

Signature :

*This application form should be returned before May 15, 1982 to
Prof. Dr. P. Phariseau, Director NATO ASI, Krijgslaan 281, S9
B-9000 GENT (Belgium).*