

# Theory and convergence properties of the screened Korringa-Kohn-Rostoker method

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Within the framework of the generalized multiple-scattering theory, a conceptually clear and transparent derivation of the real-space screened Korringa-Kohn-Rostoker method is presented. It is suggested that, by a suitable choice of the reference system, a fast exponential spatial decay of the structure constants can be obtained. This opens the way to treat large-scale systems in real space with a computational complexity that scales more favorably than the usual increase with the third power of the number of atoms.

## I. INTRODUCTION

In the past few decades, the traditional Korringa-Kohn-Rostoker (KKR) method or multiple-scattering theory<sup>1,2</sup> became a widely used computational scheme in density-functional calculations for solid matter. Many applications have been reported for the electronic structure of crystalline materials, impurities, alloys, metallic clusters, surfaces, and interfaces. As a matter of fact, multiple-scattering theory seems to be the most versatile method suited for complex atomic arrangements. However, for large-scale systems the method has been of very limited use because of its computational complexity due to the long range of the structure constants that appear in the theory. For large systems, tight-binding (TB) methods seem to be better suited. Among these the most sophisticated one is Andersen's linear-muffin-tin-orbital (LMTO) version.<sup>3</sup> It is the aim of this paper to show that the KKR method can also be transformed into a TB form. The transformation is exact and the transformed structure constants can easily be calculated in real space. By a suitable choice of the transformation, the structure constants are made to decay exponentially fast in space and this fact can be exploited to develop an order- $N$  method for density-functional electronic-structure calculations of surfaces and interfaces.

Previous work to improve the spatial decay of the KKR structure constants was based on the screening concept introduced in Ref. 3. Short-ranged screened structure constants were defined by an *a priori* transformation, the parameters of which were obtained in terms of tedious optimization procedures. In an attempt to facilitate the

original one by Andersen *et al.*,<sup>4</sup> which seemed to be rather hard to carry out for structures being more complicated than periodic lattices of cubic symmetry, Szunyogh *et al.*<sup>5</sup> recently suggested an *ad hoc* prescription for approximate optimization and developed a screened KKR method with emphasis to study metallic surfaces. Extensions including relativistic<sup>6</sup> and also spin-polarized relativistic effects<sup>7,8</sup> indicated the large variety of possible applications of the method. However, a coherent theoretical background, whether an appropriate localized representation always existed, was not provided and the optimization procedure was still rather tedious. Very recently, Andersen *et al.*<sup>9</sup> proposed a version of the LMTO method based on unitary spherical waves that are defined as localized impurity solutions in a hard sphere solid. By using these unitary spherical waves, Andersen *et al.*<sup>9</sup> also derived a generalized KKR formalism with structure constants being short ranged and nearly independent of energy.

In this paper we provide a physically transparent and exact derivation of a different generalized KKR formalism with suitably defined screening parameters, which can trivially be calculated. The fundamental idea being exploited is the freedom in the choice of the reference system with respect to which KKR theory can be formulated.<sup>10,11</sup> This fact has been used in many contexts before, in particular, when dealing with defects in metals.<sup>12-14</sup> In the original formulation given by Korringa,<sup>1</sup> and Kohn and Rostoker,<sup>2</sup> the reference system is free space. The important observation on which we base our theory is the fact that the free-space structure constants decay exponentially for negative energies since

no eigensolutions of the Schrödinger equation exist in free space for negative energies. For our purpose we thus need a reference system that supports no eigensolutions in the energy range relevant for solid-matter electronic-structure calculations. This range is rather narrow and approximately covers positive energies up to 1 Ry above zero. One can think of many reference systems that fulfill this condition, the one we choose consists of a constant repulsive potential  $V^r$  of about 2 Ry within the nonoverlapping muffin-tin spheres, while as usual the potential in the interstitial region between the spheres is defined to be zero. Such a reference system is easily implemented into existing computer codes since no new numerical quantities must be calculated. From first-order perturbation theory, the repulsive potential should shift all eigenstates of free space by about  $V^r \Omega_{\text{mt}} / \Omega_{\text{cell}}$ , where the volume ratio of muffin-tin volumes  $\Omega_{\text{mt}}$  to cell volume  $\Omega_{\text{cell}}$  enters.

For this choice of the reference system, we now first describe the screened KKR method, then show results of numerical investigations for a fcc lattice as a test case, and finally discuss how our screened KKR method can be used as an order- $N$  method in density-functional electronic-structure calculations for surface and interface problems.

## II. THEORY

According to standard multiple-scattering theory, the Green's function can be written in a mixed site-angular-momentum representation as

$$G(\mathbf{r}+\mathbf{R}_i, \mathbf{r}'+\mathbf{R}_j; E) = \sum_{LL'} R_L^i(\mathbf{r}; E) G_{LL'}^{ij}(E) R_{L'}^j(\mathbf{r}') + \delta_{ij} \sum_L R_L^i(\mathbf{r}_{<}; E) H_L^i(\mathbf{r}_{>}; E), \quad (1)$$

where the  $L \equiv (\ell m)$  are angular-momentum indices, and  $R_L^i(\mathbf{r}; E)$  and  $H_L^i(\mathbf{r}; E)$  are properly normalized regular and irregular scattering solutions corresponding to the potential centered at position  $\mathbf{R}_i$ .<sup>10</sup> The structural Green's function matrix  $G(E) = \{G_{LL'}^{ij}(E)\}$  can be expressed as

$$G = G^0 + G^0 t G^0 + G^0 t G^0 t G^0 + \dots = G^0 (I - t G^0)^{-1}, \quad (2)$$

in terms of its free-space counterpart  $G^0(E) = \{G_{LL'}^{ij}(E)\}$ , usually called *bare* structure constants, and of the single-site  $t$  matrices  $t(E) = \{t_{LL'}^i(E) \delta_{ij}\}$ , which become diagonal in the angular-momentum indices if muffin-tin potentials are used. For brevity, the explicit energy dependence of the matrices in (2) has been suppressed and  $I$  denotes a unit matrix in the mixed site-angular-momentum representation. The scattering-path operator  $\tau(E) = \{\tau_{LL'}^{s(0),ij}(E)\}$  (see, for example, Ref. 15 and references therein),

$$\tau = [(t)^{-1} - G^0]^{-1}, \quad (3)$$

is related to (2) through

$$G = G^0 + G^0 \tau G^0 = (t)^{-1} \tau (t)^{-1} - (t)^{-1}. \quad (4)$$

Equations (2)–(4) can easily be reformulated with respect to a new reference system  $r$ , in which new scattering centers with potentials  $V^r$  are located at the sites of the real scattering centers. If the  $t$  matrices and the structural Green's function matrix of this reference system  $r$  are denoted by  $t^r(E)$  and  $G^r(E)$ , we have similarly to (2),

$$G^r = G^0 + G^0 t^r G^0 + G^0 t^r G^0 t^r G^0 + \dots = G^0 (I - t^r G^0)^{-1}. \quad (5)$$

By introducing the difference of the  $t$  matrices

$$\Delta t = t - t^r, \quad (6)$$

we obtain for the Green's function of the real system instead of (2) the result

$$G = G^r + G^r \Delta t G^r + G^r \Delta t G^r \Delta t G^r + \dots = G^r (I - \Delta t G^r)^{-1}. \quad (7)$$

In analogy to (3), we introduce a scattering-path operator

$$\tau_\Delta = [(\Delta t)^{-1} - G^r]^{-1}, \quad (8)$$

so that  $G$  can also be expressed as

$$G = G^r + G^r \tau_\Delta G^r = (\Delta t)^{-1} \tau_\Delta (\Delta t)^{-1} - (\Delta t)^{-1}. \quad (9)$$

Therefore, once  $t^r$  and  $G^r$  are known, (7)–(9) represent a set of equations being equivalent to (2)–(4). The easiest way to see this equivalence is to rewrite (2), (5), and (7) formally as  $(G)^{-1} = (G^0)^{-1} - t$ ,  $(G^r)^{-1} = (G^0)^{-1} - t^r$ ,  $(G)^{-1} = (G^r)^{-1} - \Delta t$ , and to use the definition (6).

## III. NUMERICAL CALCULATIONS

When implementing the screened KKR method, the major step is to calculate the screened structure constants introduced in (5), which, in principle, involves the inversion of an infinite matrix. However, if all the elements  $G_{LL'}^{r,ij}$  decay fast enough as  $|\mathbf{R}_i - \mathbf{R}_j|$  increases, then (5) can be solved for a finite cluster of atomic sites.

In order to demonstrate this, we have made test calculations using clusters of repulsive muffin-tin potentials arranged on the sites of a fcc lattice with lattice constant  $a = 6.76$  Bohr radii, which is representative for Cu. If all lattice sites are occupied with the same repulsive potential  $V^r$ , being constant inside the muffin-tin spheres, the situation resembles a periodic crystal and (5) can exactly be solved by Fourier transformation except for the necessary cutoff in the angular-momentum indices. In our

tests we have chosen a cutoff value of  $\ell_{\max} = 4$ . As a first check we have varied the strength of the individual repulsive potential wells up to  $V^r = 8$  Ry and determined the bottom  $E_{\text{bot}}$  of the conduction band by density-of-states calculations from the imaginary part of the Green's function given by (5). We find  $E_{\text{bot}} = 0.73, 1.38, 2.37$ , and  $3.32$  Ry, for  $V^r = 1, 2, 4$ , and  $8$  Ry. Up to  $V^r = 2$  Ry, this compares well with the estimate from first-order perturbation theory  $E_{\text{bot}} = V^r \Omega_{\text{mt}} / \Omega_{\text{cell}}$  which gives  $E_{\text{bot}} = 0.74, 1.48$  Ry; whereas for higher values of  $V^r$  a saturation effect is seen. Below  $E_{\text{bot}}$  the imaginary part of the Green's function vanishes, which means that the structural Green's function elements decay exponentially in space.

The question is whether this decay is fast enough to allow for a real-space determination of  $\underline{G}^{r,ij}$  by using a finite cluster of repulsive muffin-tin potentials. In our test calculations, we have used clusters with 13, 19, 79, and 225 repulsive muffin-tin potentials situated at a central site and at the sites of the appropriate neighboring shells in a fcc lattice. The size of the potentials in the finite clusters was always chosen as  $V^r = 2$  Ry. To visualize the decay of  $\underline{G}^{r,ij}$  as a function of  $|\mathbf{R}_i - \mathbf{R}_j|$ , we introduce the following "partial norm":

$$N_{\ell\ell'}(|\mathbf{R}_i - \mathbf{R}_j|; E) = \frac{|E|^{(\ell+\ell')/2}}{(2\ell+1)!!(2\ell'+1)!!} \times \left[ \sum_{mm'} |G_{\ell m, \ell' m'}^{r,ij}(E)|^2 \right]^{1/2}, \quad (10)$$

with  $(2\ell+1)!! = (2\ell+1)(2\ell-1)\dots(3)(1)$ . The quantity  $N_{\ell\ell'}$  is identical within a chosen shell of neighbors, i.e., for a given distance  $|\mathbf{R}_i - \mathbf{R}_j|$  it shows no angular dependence. Note that these partial norms cannot be expanded at  $E = 0$ , a fact already seen in the zeroth-order Ricatti-Hankel function  $\exp(i\sqrt{E}r)$  with absolute value equal to one for  $E > 0$  and equal to  $\exp(-\sqrt{|E|r})$  for  $E < 0$ . The partial norms calculated with 225 sites are plotted for  $\ell = \ell'$  in Fig. 1 (left panel) as a function of the distance  $|\mathbf{R}_i - \mathbf{R}_j|$  for the choice  $E = 0.65$  Ry, which is representative for the Fermi energy of Cu. They are compared with the corresponding norms of the bare Green's function  $G^0$  in Fig. 1 (right panel). It is obvious from Fig. 1 that the partial norms corresponding to the screened structure constants  $\underline{G}^{r,ij}$  decay rapidly and essentially exponentially. Whereas the unscreened norms typically decrease by less than a factor of 10 in the distance range shown in Fig. 1, the screened norms decrease to about  $10^{-5}$  of their nearest-neighbor values. This decay extends up to the outermost sites covered with repulsive potentials and no surface effects are seen. With respect to such surface effects, the choice of our intermediate reference system with finite repulsive potential at all sites in the cluster seems to be more robust than the concept of unitary spherical waves,<sup>9</sup> where infinite repulsive potentials are used in the cluster except for the central site and where as a consequence surface states can tunnel in if the cluster is too small.

If the screened partial norms are plotted as function of energy (see Fig. 2 for  $\ell = \ell' = 0$  and Fig. 3 for

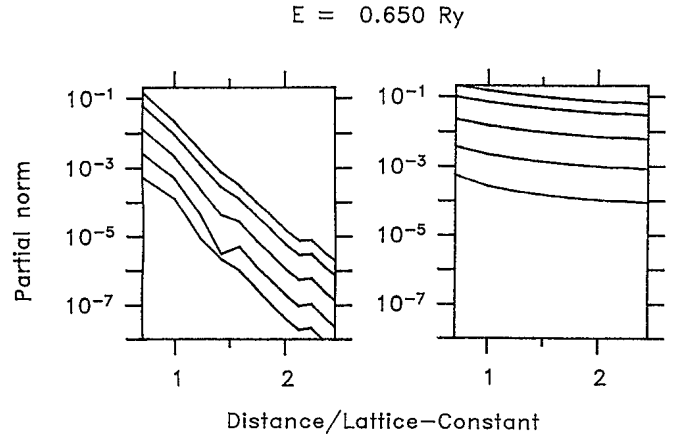


FIG. 1. Screened (left panel) and unscreened (right panel) partial norms for  $\ell = \ell'$  and  $E = 0.65$  Ry as a function of the distance in units of the lattice constant. The results for  $\ell = 0, 1, 2, 3$ , and  $4$  are shown from top to bottom.

$\ell = \ell' = 2$ ), two observations can be made. The decay of the screened structure constants is very similar in the relevant positive energy range of about 1 Ry and calculations with clusters of 79 or 225 repulsive muffin-tin potentials lead to almost indistinguishable results as far as the distance  $|\mathbf{R}_i - \mathbf{R}_j|$  does not extend beyond the range of repulsive potentials. (Only results for these distances are plotted in Figs. 2 and 3.) The conclusions that can be made from Figs. 2 and 3 are that because of the smooth energy dependence, the screened structure constants can easily be interpolated with respect to energy and that they can be calculated by using rather small clusters. Both facts can be exploited to speed up the calculations and this is true even up to energies less than 0.4 Ry below the conduction-band bottom  $E_{\text{bot}}$  of the reference system. If, of course, the energy approaches  $E_{\text{bot}}$ , which is 1.38 Ry for our choice  $V^r = 2$  Ry, then the exponential decay breaks down and the screened structure constants become strongly energy dependent. However, such

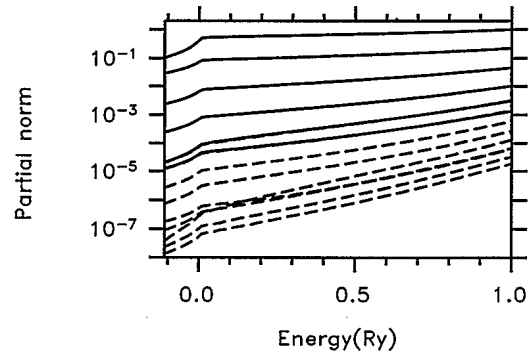


FIG. 2. Screened partial norms for  $\ell = \ell' = 0$  as a function of energy. From top to bottom on-site results and the ones for 12 neighboring shells with increasing distance from the central site are given. The 6 solid curves are calculated with repulsive potentials on 79 sites, the 13 broken curves with 225 sites. (The 6 upper broken curves practically coincide with the solid ones.)

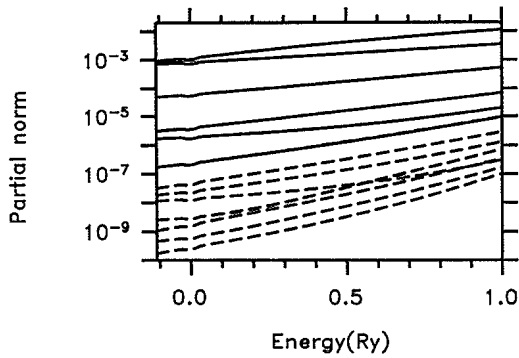


FIG. 3. Screened partial norms for  $\ell = \ell' = 2$  as a function of energy. From top to bottom on-site results and the ones for 12 neighboring shells with increasing distance from the central site are given. The 6 solid curves are calculated with repulsive potentials on 79 sites, the 13 broken curves with 225 sites. (The 6 upper broken curves practically coincide with the solid ones.)

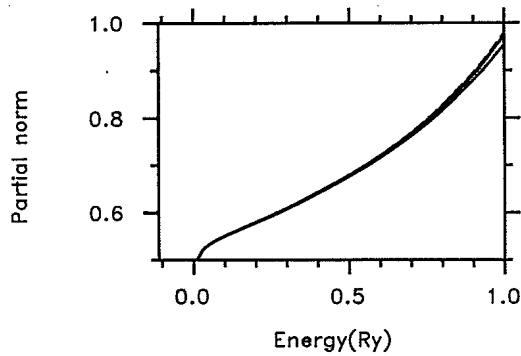


FIG. 4. On-site screened partial norms for  $\ell = \ell' = 0$ . The lower solid curve is calculated with 13 repulsive potentials, the upper solid curve with 19 ones, and the almost indistinguishable broken curve with 225 ones.

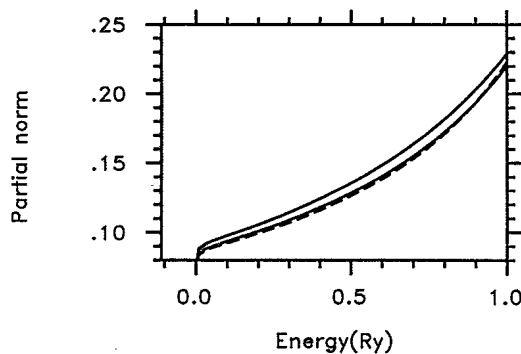


FIG. 5. Screened partial norms for the first-neighbor distance and for  $\ell = \ell' = 0$ . The upper solid curve is calculated with 13 repulsive potentials, the lower solid curve with 19 ones, and the broken curve with 225 ones.

energies do usually not occur in self-consistent density-functional calculations for occupied states and, if they do, one could increase  $V^r$  to, say, 3 or 4 Ry (see above) to extend the energy range of fast decaying and smoothly varying screened structure constants. Since the curves in Figs. 2 and 3 are plotted on a logarithmic scale covering several orders of magnitude, the small differences obtained between the clusters of 79 or 225 repulsive potentials are difficult to see since both curves practically coincide. For that reason we plot the partial norms for  $\ell = \ell' = 0$ , where these differences are largest, on a magnified linear scale in Fig. 4 showing the on-site norm and in Fig. 5 showing the one for the first-neighbor distance as calculated with repulsive muffin-tin potentials on 225, 19, and 13 sites. Whereas the on-site results are practically identical for 225 and 19 sites, small differences for first-neighbor results are seen, even if 19 sites and 225 sites are compared, but these small differences may well be neglected in real calculations.

#### IV. ORDER- $N$ METHODS

As it was mentioned in the beginning of this paper, the screened KKR method has already been applied for surface and interface problems where the short-ranged behavior of  $\underline{G}^{r,ij}$ , the structure constants in the screened representation, was fully exploited. Even with the not too well screened structure constants obtained by the prescription given in Ref. 5, the calculated results were very satisfying.<sup>5-8</sup> Therefore, it is reasonable to assume that the new screened structure constants obtained by our method of an intermediate reference system can fairly well be neglected after nearest or next-nearest neighbor distances. As a consequence, already demonstrated in Figs. 2 and 3, the screened structure constants can be calculated for each site *independently* by solving matrix equation (5) with matrix dimensions given by the product of the number of angular momenta and the number of neighboring sites taken into account. Thus, the calculation of  $\underline{G}^r$  is an  $O(N)$  problem for systems with  $N$  sites and the linear scaling begins to apply already for small systems with about 20 sites.

Whereas the reference Green's function  $\underline{G}^r$  must be calculated only once, the calculation of the real Green's function  $\underline{G}$  must be repeated in each self-consistency iteration cycle. This second step requires the solution of (7) or (8) where the matrices  $I - \Delta t \underline{G}^r$  or  $(\Delta t)^{-1} - \underline{G}^r$  are of block-sparse form. The number of blocks grows linearly with system size since  $\underline{G}^r$  decays exponentially and can be cut after a chosen range of interactions. The individual blocks are matrices with angular-momentum indices and the blocks are labeled by site indices. If a complex energy contour<sup>16</sup> is used to calculate the electronic density from the structural Green's function elements  $G^{ij}(E)$  of the real system and *if* these elements decay rapidly with distance as in insulators, semiconductors (and for most of the complex energies in metals), they can be neglected after a chosen distance. Then the situation is similar to our reference system and the complete calculation is an  $O(N)$  problem for systems with

$N$  sites, but linear scaling only applies for larger systems with more sites since the decay in the real physical system is normally slower than in our reference system.

If the elements  $G^{ij}(E)$  cannot be neglected for larger distances because they decay too slowly as in metals for complex energies close to the Fermi energy, nevertheless one should be able to exploit the sparsity of the matrices  $I - \Delta t \mathbf{G}^r$  or  $(\Delta t)^{-1} - \mathbf{G}^r$ . This is probably most efficiently done by iteration techniques like the recursion method. The attainable accuracy and the overall computational complexity of iterative techniques for general three-dimensional systems is not straightforwardly assessed and requires further investigations. For surface and interface problems, the situation is much simpler since the two-dimensional periodicity allows for two-dimensional Fourier transformation. This simplifies the form of the matrices from *block sparse* into *block banded* with a bandwidth given by the number of interacting layers in the intermediate reference system. It is well known that direct solutions of linear systems of equations with band matrices is an  $O(N)$  problem. On first sight, the direct solution of (7) or (8) in order to obtain  $\mathbf{G}$  or  $\tau_\Delta$  seems to require matrix inversions, that is to solve  $O(N)$  equations, each with  $O(N)$  complexity, resulting in an  $O(N^2)$  problem. However, only the diagonal blocks of  $\mathbf{G}$  or  $\tau_\Delta$  are needed to construct the electronic density in density-functional calculations and one can simplify the calculations into an overall  $O(N)$  problem by algorithms as given, for instance, by Godfrin<sup>17</sup> and Wu and co-workers.<sup>18</sup>

It is important to point out here that our  $O(N)$  screened multiple-scattering method for surface and interface problems is free from uncontrolled approximations. The method is essentially exact except for the usual, controllable cutoff in angular momentum and the equally controllable cutoff in the screened structure constants that decay rapidly with  $|\mathbf{R}_i - \mathbf{R}_j|$ . Since only nearest or next-nearest layers interact in our reference system, the break-even point, where one can profit from the linear scaling with system size, already occurs for a small number of layers, say three or five. It is also important to point out that the rapid, exponential decay is not a property of the physical system of interest but of the intermediate reference system. Thus our  $O(N)$  multiple-scattering method is equally applicable for surface and interface calculations of insulators, semiconductors, and metals. We may remark here that, in principle, an  $O(N)$  method to solve the Schrödinger (Kohn-Sham) equation should be combined with an  $O(N)$  method to solve the Poisson equation. Such methods exist like the fast multipole method of Greengard-Rokhlin.<sup>19</sup> In practice, standard schemes as given by Schädler<sup>20</sup> or Gonis *et al.*<sup>21</sup> seem to be equally well suited since the  $O(N^2)$  overhead to solve the Poisson equation by these schemes is negligible for the number of sites that can be used on today's computers in self-consistent density-functional calculations.

## V. DISCUSSION

Real-space methods for electronic-structure calculations of large, complex systems have gained increasing

popularity in recent years as one can see from the many successful applications of the TB-LMTO method. In some respects the screened KKR method is similar to the TB-LMTO method. Both methods are very economical since the potential and structural information are elegantly separated and since usually 16 angular-momentum indices are enough because of the centrifugal barrier  $\ell(\ell + 1)/r^2$  in the radial Schrödinger equation. Both methods are all electron methods equally applicable to any atom from the periodic table and there is no ambiguity in the choice of basis functions or in the construction of a pseudopotential with unknown transferability properties. Both methods contain universal screening parameters (the energy-dependent single-site  $t$  matrices  $t^r$  of the reference system correspond to the energy-independent  $\alpha$  parameters in the TB-LMTO method) and allow us to account for full-potential effects in a straightforward manner. The two main advantages of our screened KKR method are the ease with which the screening parameters and the resulting screened structure constants can be calculated and the property that the method is derived by an exact transformation without any approximations. From a computational point of view, the screened KKR method requires matrix inversion (solution of linear equations) for each energy on the complex energy contour, whereas the TB-LMTO method with the inherent linearizing step leads to an eigenvalue problem that is solved only once. Since usually 20 to 40 energy mesh points are enough and since solutions of linear equations are faster than eigenvalue determinations, the computational work should be comparable.

In conclusion, we have presented an exact transformation of the multiple-scattering (KKR) method into a tight-binding-like form with screened structure constants that decay rapidly and are easily calculated in real space. The transformation is based on the use of an intermediate reference system with repulsive muffin-tin potentials and leads to universal screening parameters uniquely defined by the radius of the muffin-tin spheres and the magnitude of the repulsive reference potentials. The method can be used in real space as already demonstrated by a number of applications.<sup>5-8</sup> For surface and interface problems, the computational complexity scales linearly with the number  $N$  of layers taken into account. Compared to the conventional  $N^3$  scaling, this leads to considerable savings in computer time, a fact that can already be exploited if more than three or five layers are used. For arbitrary three-dimensional situations, the savings in computer time are also substantial because of the sparsity of matrices, but the question of suitable algorithms and their computational complexity is not easily answered and remains a subject of future research.

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