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大規模スーパーセルを対象とした遮蔽 KKR 法に基づく第一原理計算コードの開発

Title: Development of a first-principles code for large super-cells based on the screened KKR method

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The KKR Green's function method is a method for first-principles electronic structure calculations. In this method, instead of solving eigenvalue problems, Green's function of the Kohn-Sham equation is directly calculated. By taking the imaginary part of the Green's function, we can obtain the electron density very accurately and efficiently.

The Green's function is calculated from that of an arbitrary reference system by solving the Dyson-type equation. In the process of solving the Dyson equation, inversions of matrices of a dimension proportional to N (N: the number of atoms in a unit-cell) is required. In the usual KKR method, the free space is chosen as the reference system. When N becomes large, the computational cost increases drastically. This is because $O(N^3)$ operations are required to invert a $N \times N$ matrix. To overcome this difficulty, the concept of screened KKR was proposed. In the screened KKR method, a system with repulsive muffin-tin potentials of a constant height is chosen as the reference system. In this reference system, the Green's function decays exponentially in real-space if the energy range is sufficiently lower than the repulsive potential height. Then we can ignore long range propagations without sacrificing the accuracy. In this case, the matrix that we must invert becomes sparse. Therefore, one can expect large improvement of the calculational efficiency by use of an efficient sparse matrix solver. This technique has been mainly applied to the multilayered systems which extend to only one dimensional direction assuming two-dimensional periodicity. For such systems, the matrix becomes block tridiagonal and the computational cost is exactly proportional to the layer thickness.

It is desirable to apply the screened KKR technique to more general and complex systems which extend to all three dimensional directions. For such general large super-cells, we must treat general non-Hermitian block sparse matrices. As a sparse matrix solver, the iterative method, which is often used to solve linear simultaneous equations with sparse coefficient matrices, is more efficient than the direct method such as the *LU*-factorization. This algorithm is suitable for the parallel computing.

We developed a full-potential based screened KKR code which can treat such large super-cells by combining the iterative method for solving the Dyson equation with parallel computing techniques. Through the test calculations, it is shown that our code is reliable and well parallelized w.r.t the number of atoms in the super-cell. By the use of our code, it is possible to execute the all-electron level first-principles electronic structure calculations for super-cells which include thousands of atoms within a reasonable time.