Poster

# First-principles Calculation Method for Electronic Structures of Nanostructures Intervening between Semi-infinite Electrodes

Takashi Sasaki, Tomoya Ono, and Kikuji Hirose
*Department of Precision Science and Technology, Osaka University, Osaka 565-0871, Japan*
E-mail: t-sasaki@cp.prec.eng.osaka-u.ac.jp
http://www-cp.prec.eng.osaka-u.ac.jp/

The prospect of being able to predict and explain the property of condensed matter systems at the atomic level, by solving the fundamental equations for nuclei and electrons based on the density functional theory [1], has attracted much attention from many generations of scientists since the early days of quantum mechanics.

A number of first-principles calculation techniques employing basis sets have been developed in the past [2-4]. Although these methods have been used with great success, there are a few serious drawbacks. For example, the completeness of the basis set is always a concern, and treating nonperiodic systems with the plane wave basis leads to the waste of computational effort.

A method which solves the Kohn-Sham equation directly on grid points in the real space has recently been introduced[5-10], which avoids many of these problems. Within this method, boundary conditions are not constrained to be periodic, which permits the use of nonperiodic boundary conditions for clusters and a combination of periodic and nonperiodic boundary conditions for surfaces. Furthermore, in order to realize the order-$N$ ($O(N)$) calculation, the orbitals constrained to be localized in finite regions of the real space can be employed instead of wave functions extending over supercells, and then, by making efficient use of the advantages of such localized orbitals, one can calculate the ground-state electronic structure of a nanostructure sandwiched between two infinitely continuing crystalline electrodes (see Fig. 1 for an example).

In this study, we have developed a first-principles procedure for electronic structure calculations of nanostructures suspended between crystalline electrodes, in which the real-space finite-difference method [5-10] and the localized-orbital technique [11, 12] are combined. Directly minimizing [13] the energy functional proposed by Mauri, Galli and Car [14], we obtain satisfactorily the self-consistent solutions of the Kohn-Sham equation without usage of conventional self-consistent field techniques. We apply this method to electronic structure calculations for single-row gold wires, and by evaluating their electronic conductance, we verify the accuracy and applicability of this method.

As numerical examples, we demonstrated the electronic structure and conductance calculations of the single-row gold wires sandwiched between electrodes. From the results that the calculated conductance is consistent with that obtained by experimental and other theoretical studies, it seems reasonable to conclude that our procedure is suitable for electronic structure calculations of a nanostructure suspended between electrodes (Fig. 2).

In addition, when a system is assumed to be described in terms of localized orbitals, this procedure makes it possible to perform the calculation with linear system-size scaling $O(N)$. The linear scaling method is promising frameworks for the study of broader structures than affordable with conventional techniques. Research in this direction is in progress.

**References:**

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**Figures:**

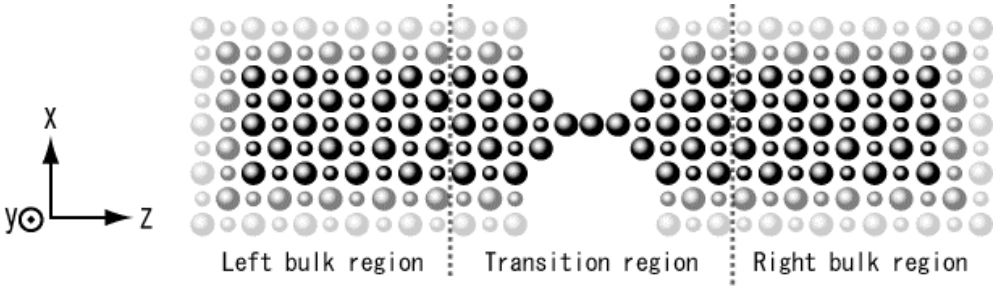


Fig. 1 Schematic representation of the wire system for L=1 with the transition region suspended between the left and right bulk regions. The large and small spheres represent the atoms on and below the cross section, respectively.

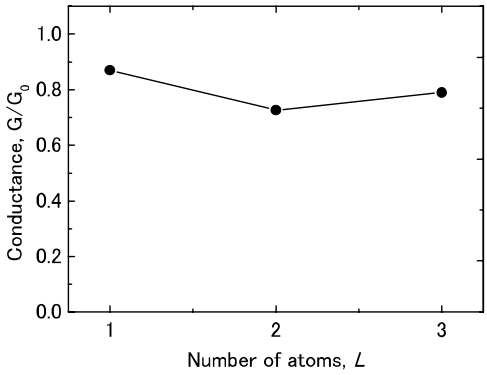


Fig. 2 Conductance of the atomic wires in units of the conductance quantum ($G_0$) as a function of the number of gold atoms in the wire.