# Efficient electronic structure calculation in the mixed basis approach

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To find the solution of the Kohn-Sham (KS) equation requires the iteration procedure until the electron density generated by an effective one-particle potential is identical to the one used to create the potential. In the self-consistent calculation, the calculation of the KS Hamiltonian matrix elements (i.e., numerical integrations) should be performed in each iteration. The evaluation of the matrix elements is a formidable task when a number of basis functions are needed to solve the KS equation. This is an obstacle to the fast electronic structure calculation. Thus, development of an efficient algorism is mandatory.

In this work, we propose an algorism for calculating the Hamiltonian matrix elements. The procedure is as follows: (i) Before starting the self-consistent calculation, calculate the matrix elements with regard to the Chebyshev polynomials. (ii) In each iteration, fit the KS potential by the Chebyshev polynomials. (iii) Express the KS Hamiltonian matrix elements by a linear combination of the matrix elements with regard to the Chebyshev polynomials. This approach reduces the numerical cost in the self-consistent calculation because a lot of numerical integrations are replaced by just the KS potential fitting procedure mentioned in (ii). We expect that the accuracy of this approach may be good because it is known that the error of the Chebyshev approximation is smaller than that caused by the use of the other orthogonal polynomials [1]. We performed a benchmark calculation of the electronic structure of Si bulk crystals and carbon-related nanomaterials by all-electron mixed basis *ab initio* program TOMBO that will be available as open-source software in the near future. We used 4 cores of the HITACHI SR16000 at Hokkaido University.

Figure 1(a) shows the setup time for the matrix as a function of nw that is the number of the plane waves used in the electronic structure calculation of a fullerene molecule. If we perform numerical integrations to calculate the KS Hamiltonian matrix elements, the sum of the time spent on it for each self-consistent cycle is ~30s for nw~40000. However, using the above prescription only 3 seconds are required. Figure 1(b) shows the HOMO energy of a fullerene molecule as a function of Mcheb, the number of the Chebyshev polynomials. The HOMO energy within the Chebyshev approximation are in agreement with that computed by numerical integration to more than 99.999% accuracy when we used more than 20 Chebyshev polynomials. These results demonstrate that the proposed method is practical for performing efficient and accurate electronic structure calculations in TOMBO.

[1] W. M. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes in Fortran 90: The Art of Parallel Scientific Computing* (Cambridge University Press, 1996).

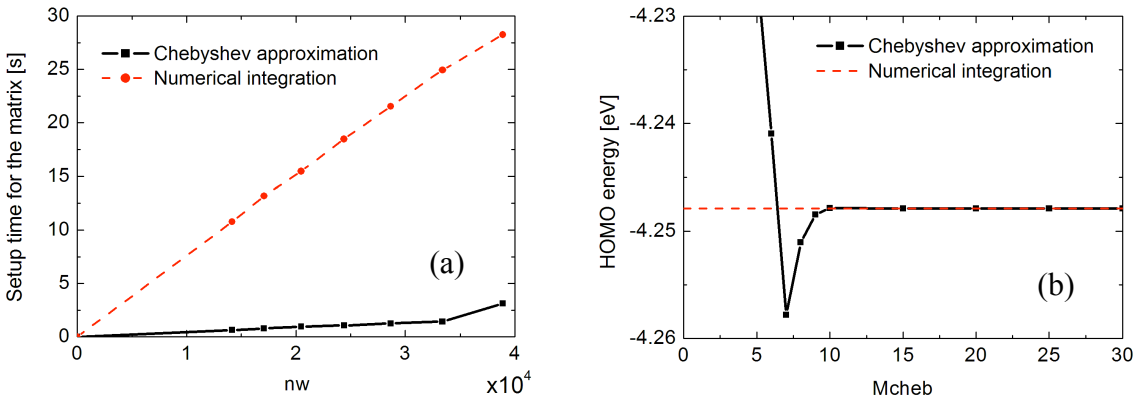


FIG. 1: (a) nw-dependence of the setup time for calculating the KS Hamiltonian matrix elements in the electronic structure calculation of a fullerene molecule, where nw is the number of the plane waves used in the calculation. (b) HOMO energy of a fullerene molecule as a function of Mcheb that is the number of the Chebyshev polynomials used in the calculation.