

Tutorial of TOMBO Ver. 2.0

090731 version





What is TOMBO ?

TOhoku **M**ixed-**B**asis **O**rbital *ab initio* program “TOMBO”, which has been developed by our research group, is a tool for the first principles calculations based on “all-electron mixed basis approach” [1-3].

[1] K. Ohno, K. Esfarjani, and Y. Kawazoe, Computational Materials Science: From ab initio to Monte Carlo Methods, Springer Series in Solid-State Sciences Vol. 129 (Springer-Verlag, Berlin, Heidelberg, 1999), 42-46.

[2] M. S. Bahramy, M.H.F. Sluiter, and Y. Kawazoe, Phys. Rev. B **73** (2007), 045111.

[3] <http://www-lab.imr.edu/~tombo/>



Formation and advantages:

One-electron wave function is expressed as:

◎ All-electron:

Core
Valence

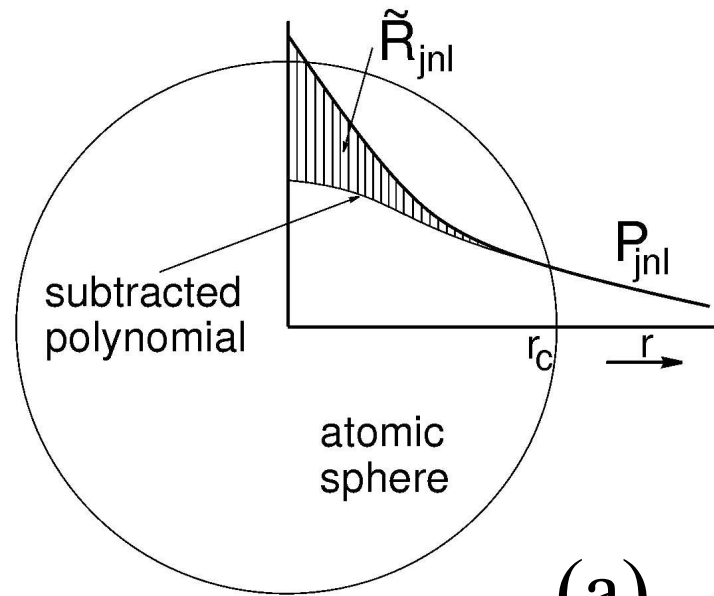
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◎ Mixed-basis approach:

Atomic orbitals (AO)
Plane wave (PW)

◎ Reduction of number of PW, which is necessary for standard planewave based approaches.

◎ Study of properties affected by core level such as XPS and hyper fine structures [2].



(a)

$$\begin{aligned}
 \Psi^\lambda(\mathbf{r}) &= \sum_{\mathbf{G}} c_{\mathbf{G}}^\lambda \frac{e^{i\mathbf{G}\cdot\mathbf{r}}}{\sqrt{\Omega}} + \sum_j \sum_{nlm} c_{jnlm}^\lambda \Phi_{jnlm}(\mathbf{r} - \mathbf{R}_j) \\
 &= \underbrace{\sum_{\mathbf{G}} c_{\mathbf{G}}^\lambda |\mathbf{G}\rangle}_{\text{PW basis set}} + \underbrace{\sum_j \sum_{nlm} c_{jnlm}^\lambda |\Phi_{jnlm}\rangle}_{\text{AO basis set}}
 \end{aligned}$$

(b)

Figure 1. (a) Construction of AOs from atomic radial wave function and (b) Kohn-Sham wave functions.



Tutorial : drawing the total charge density of CH₄ (LDA)

1. Input files
2. Output files
3. Drawing the charge density using TOMBO module with AVS/Express
4. Notes for setting parameters
5. Notes



1. Input files

Input files: defaults.in, atomicdata.in, atomxyz.in, inputdeck.in

For CH₄ (LDA), you can download a set of all the input and output files from the following URL:

<http://www-lab.imr.edu/~tombo/CH4.tar.gz>

cf. The other example is LSDA calculation of O₂.

See <http://www-lab.imr.edu/~tombo/O2.tar.gz>



2. Output files

You will obtain the following output files after calculation: atomxyz.out, avs001.out, error.out, inputdeck.out, log.out, trajectory.out, and also restart.out.

(In the present samples, restart.out is not included)

The explanation for each input and output files can be seen in the manual, pp. 35-48.

Please download the manual from the following URL:

<http://www-lab.imr.edu/~tombo/manual090105.pdf>



3. Drawing charge density using TOMBO module with AVS/Express

It is necessary to prepare two files, avs001.out and corresponding POTCAR file (VASP).

Prepare POTCAR file, whose data are used for distinguishing atom species properly. Sequential of atomic species of potential table in POTCAR file should be same in atomxyz.in

You can download a manual of TOMBO module from the following URL:

http://www-lab.imr.edu/~kazu/avs/manual/jpn/AVS-basic-man_ver2.3j.pdf

See chapter 4 (p.9) in detail. (Japanese only)



4. Notes for setting parameters

Some parameters (mesh size and cut-off energy, etc.) in `inputdeck.in` may be changed automatically to be suitable for calculating. Therefore be careful especially when you use two different types of platforms. This is because a platform dependent code (fast Fourier transform (FFT)) use different basis set depending on the platform, and some parameters of TOMBO depend on the value. The parameters used for calculation can be seen in `inputdeck.out`.



5. Notes

The present version of TOMBO is NOT suitable for using GGA.



Contact address

If you have any questions for using TOMBO Ver. 2.0, please contact us.

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