How to download?

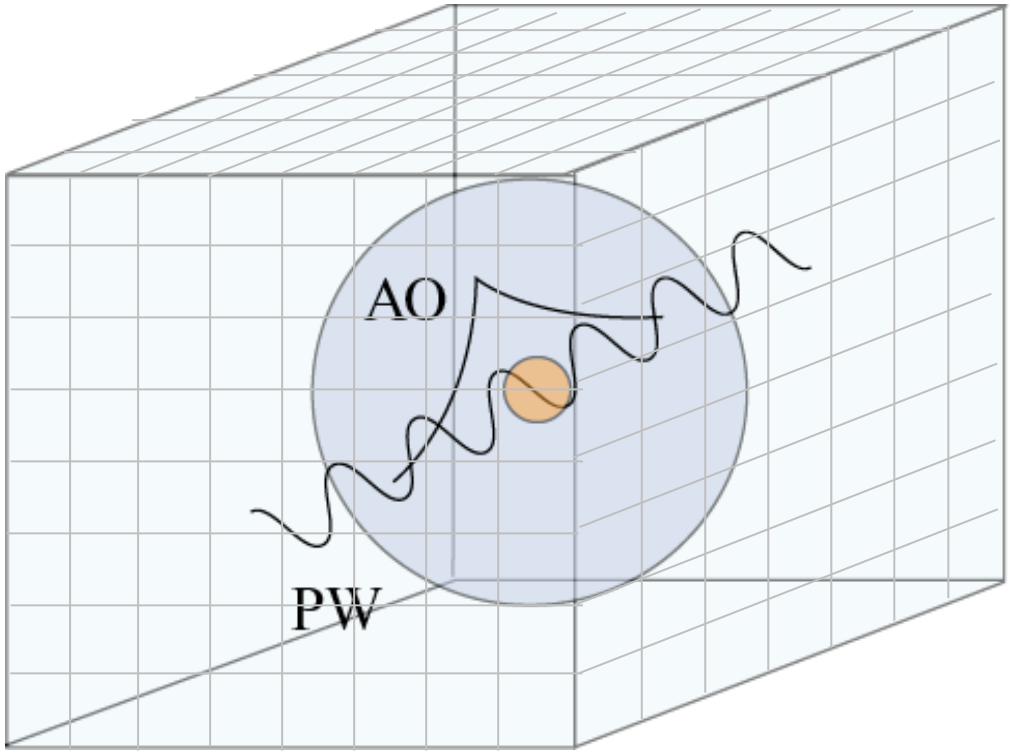
TOMBO Ver.2

All-electron mixed basis approach: TOMBO

$$\psi_\nu(r) = \sum_{\boldsymbol{G}} c_{\boldsymbol{G}}^{\nu} e^{i(\boldsymbol{G}+\boldsymbol{k})\cdot\boldsymbol{r}} + \sum_{m} c_m^{\nu} \varphi_m^{\mathrm{Bloch}}(\boldsymbol{k},\boldsymbol{r})$$

Plane Wave (PW)

Bloch Function of AO



$$\varphi_m^{\mathrm{Bloch}}(\boldsymbol{k},\boldsymbol{r}) = \sum_{n} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_n} \varphi_m^{\mathrm{AO}}(\boldsymbol{r}-\boldsymbol{R}_n)$$

Atomic Orbital (AO)

LDA and GW calculations are available using TOMBO Ver.2

- all-electron LDA calculations and MD simulations
- TDDFT excited-state dynamics simulations
- all-electron *GW* calculations for photoelectron spectra
- Bethe-Salpeter equation for photoabsorption spectra
- Hartree-Fock and self-consistent *GW*, etc.

- Hyperfine ・・・ coming in the future
- NMR ・・・ coming in the future
- van der Waals ・・・ coming in the future
- GWΓ ・・・ coming in the future

TOMBO interface using Materials Studio© & Pipeline Pirot©

DASSAULT SYSTEMES

BIOVIA

http://www.ohno.ynu.ac.jp/tombo/index.html

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What is TOMBO? Download

Tutorial Document Download

Tutorial INPUT Files Download

Manual for LDA & GW Calculations Download

LDA Source Code
(License Agreement and Registration Required)

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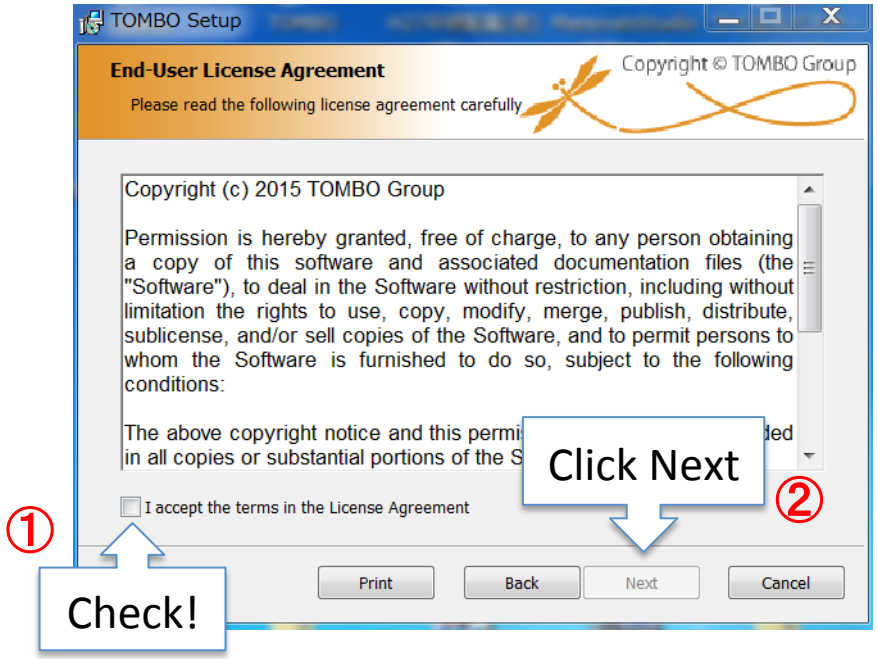
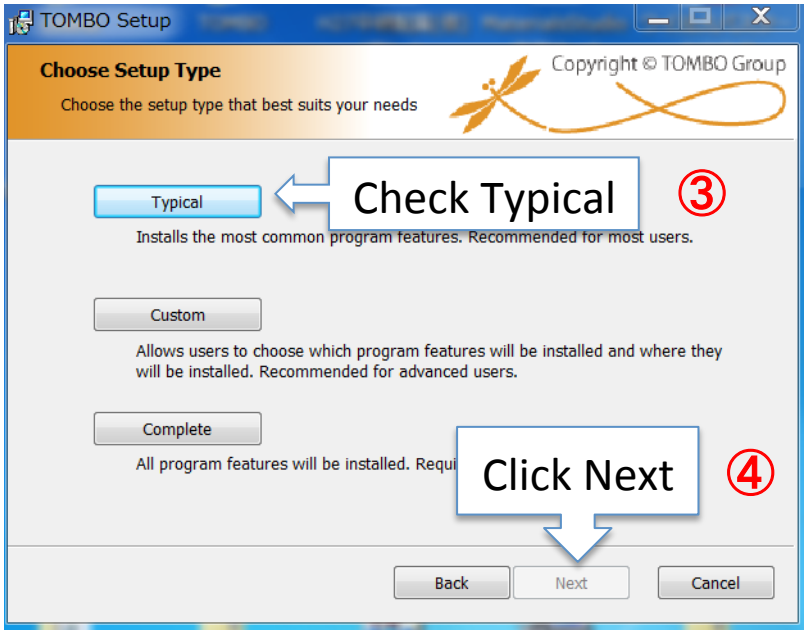
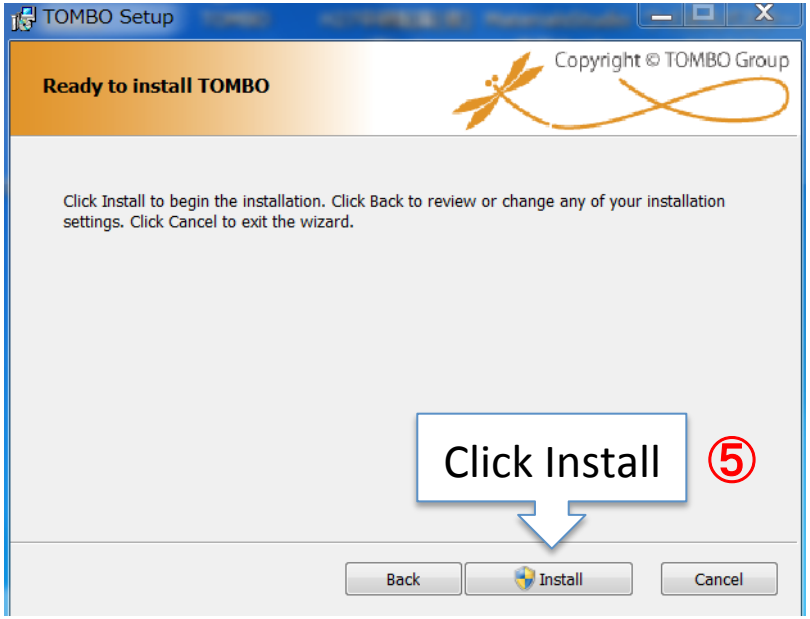
TOMBO.msi

Examples

Download from WEB to Desktop on your PC







⑦ **Reboot your PC**

Open COMMAND PROMPT

cd Documents
cd TOMBO
cd Examples
dir

type

```
2015/11/03 10:36  <DIR>      .
2015/11/03 10:36  <DIR>      ..
2015/11/03 10:36  <DIR>      CO2+2H_MD
2015/11/03 10:36  <DIR>      Li2_GW+BSE
2015/11/03 10:36  <DIR>      Si_GW
2015/11/03 10:36  <DIR>      Si_LDA
Examples>
```

cd => one of the CO2+2H_MD, Li2_GW+BSE, Si_GW, Si_LDA directories
Type TOMBO and press the “ENTER” key.
For multicore PC (e.g. 2 cores), type TOMBO –np 2 or TOMBO /np 2
After the job finished, look at *.out files by using more or word pad.

See “TOMBO Ver.2 tutorial.pdf” for more detail.

LDA Source Code (License Agreement and Registration Required)

(1) This Source Code is open for academic use only. Any commercial use is strictly forbidden. However, not only academic people (students and researchers) but also company people can download this Source Code.

(2) Anyone who uses this Source Code cannot distribute it or its modified version to anyone else.

(3) If you find any bug or problem, please send the detail information to TOMBO group (tomobo@ynu.ac.jp).

(4) TOMBO group can use the registered information for support if necessary, but does not use it for any other purpose.

AGREE

REFUSE

AGREE  https://career.phys.ynu.ac.jp/tombo/

TOMBO GROUP

TOMBO download/support WEB

User ID

Password

login

Registration Forget ID/PW

79-5 Tokiwadai, Hodagaya, Yokohama 240-8501, Japan

TOMBO GROUP

Please input your data:

Name*	First Name	Middle Name	Last Name
Position*			
Affiliation*			
City*			
Zip Code*			
Country*			
Telephone*			
E-mail*			

*are necessary items

Next

<<Exit

79-5 Tokiwadai, Hodagaya, Yokohama 240-8501, Japan

TOMBO GROUP

Input your Password

New PW

Retype New PW

Register

Stop/Exit

79-5 Tokiwadai, Hodagaya, Yokohama 240-8501, Japan

TOMBO GROUP

Your ID was assigned

TU4558

Please remember this ID and PW for your later use.

If you forget your ID, contact

tombo@ynu.ac.jp

OK

79-5 Tokiwadai, Hodagaya, Yokohama 240-8501, Japan

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ID:Name	TY0947 : Taro Yokohama	Update Personal Info.	LOGOUT

year 2015 ^ v

- TOMBO LDA Source Code Download
- Upload your modified code & your message
- Information on a k-point generator for TOMBO

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- 2015-11-01 12:03:29 [TOMBO Support] To download the TOMBO Ver.2 LDA source code, click TOMBO_Ver2_2015_11_10.zip:
  Download File>> TOMBO_Ver2_2015_11_10.zip

Whenever you modify the code, you are requested to upload your modified code from The other sheet "Upload your modified code & your message."

If you have comment to be seen to all users, please write a comment in the following Column and press "Send" button. Your name will be hiden but you can write your initial (nickname or full name) in your message if you like.

Comment:

Send

After download, please read README.txt first.
There are several Makefiles for gfortran,
INTEL fortran compiler, and supercomputers.

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Please use TOMBO

http://www.ohno.ynu.ac.jp/tombo/index.html

If you have a question, send an email to

tombo@ynu.ac.jp