Recent progresses on MULTIBINIT, ABINIT-Wannier90 interface,Lattice Wannier functions, and TB2J

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Updates on 

New features, optimisations, and bug fixes

New features:

- Adding weights to training set for improved fitting of low energy states
- External electric field.
- Selecting the “nbody” terms.
- Improved method for the selection of the bounding terms.
- Method for building superlattices

MULTIBINIT is now more stable.
Many models have been produced!

Optimizations:

- Much faster high-order term generation.
- Faster term selection with new strategies

Bug fixes:

- symmetry problem in generation of some higher-order term.
- Correction to the forces in strained structure.

Work with L. Bastogne, A.Sasani, HZ. Zhang, Ph.Ghosez

Updates on  - WANNIER90

ABINIT-Wannier90 interface

- Refactoring the ABINIT-w90 interface by using the high-level wfd_t.
- Wannierization can now run as a wfk_task.
- It can read wave functions in IBZ and generate BZ wave functions.
- The conventional way of wannierization can be used too.
- Optimisation are still needed.

Example:

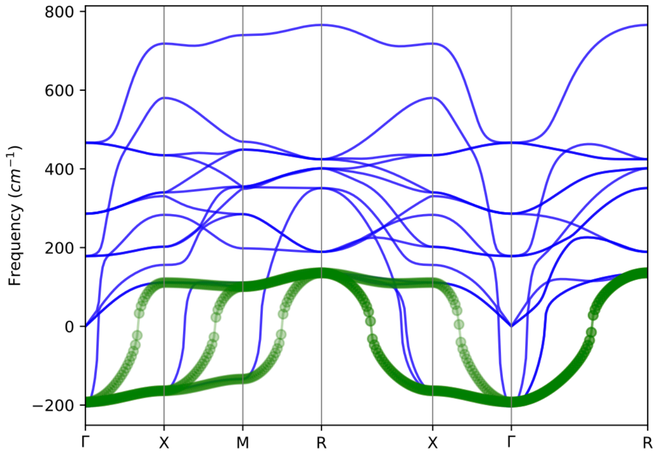
```
 ndtset  2
 ngkpt  2  2  2
……
# First dataset : SCF run with kpoints in the IBZ
 kptopt1 2

# dataset 2. Use wfk_task wannier for the wannierization
 optdriver2 8
 wfk_task2 "wannier"
 getwfk2   -1   # Read WKF in the IBZ
 prtwant2 2
 w90iniprj2 2
 kptopt 2
```

With M. Giantomassi & M. Verstraete

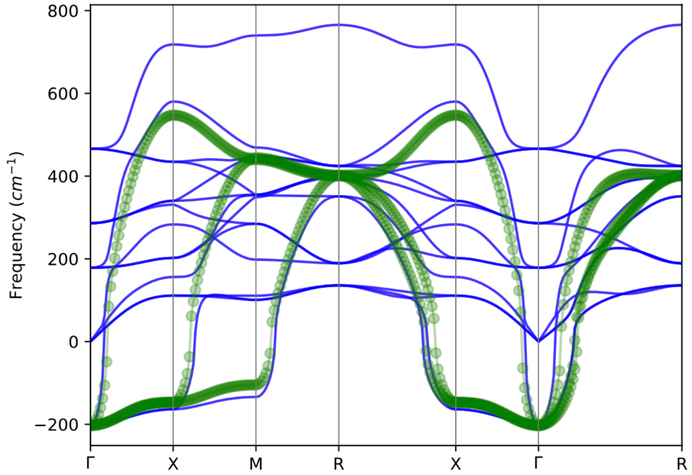
Updates on  LaWaF

LaWaF: build lattice Wannier function with ease

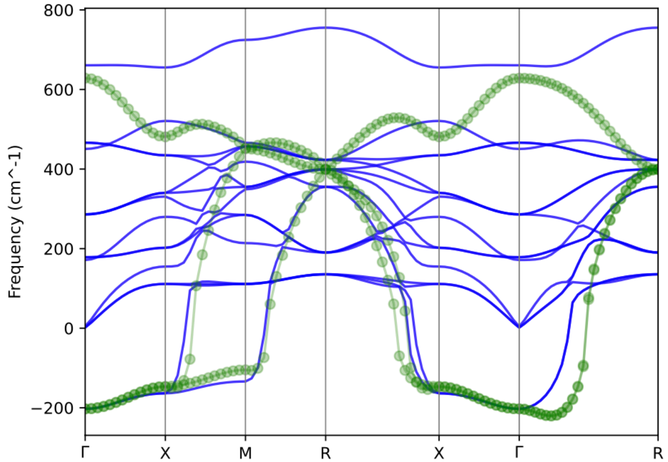
SCDM-k



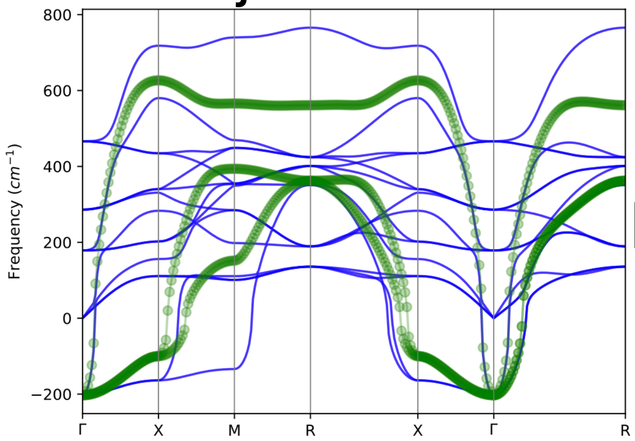
Projection+SCDM-k



Dipole-dipole



Projected WF

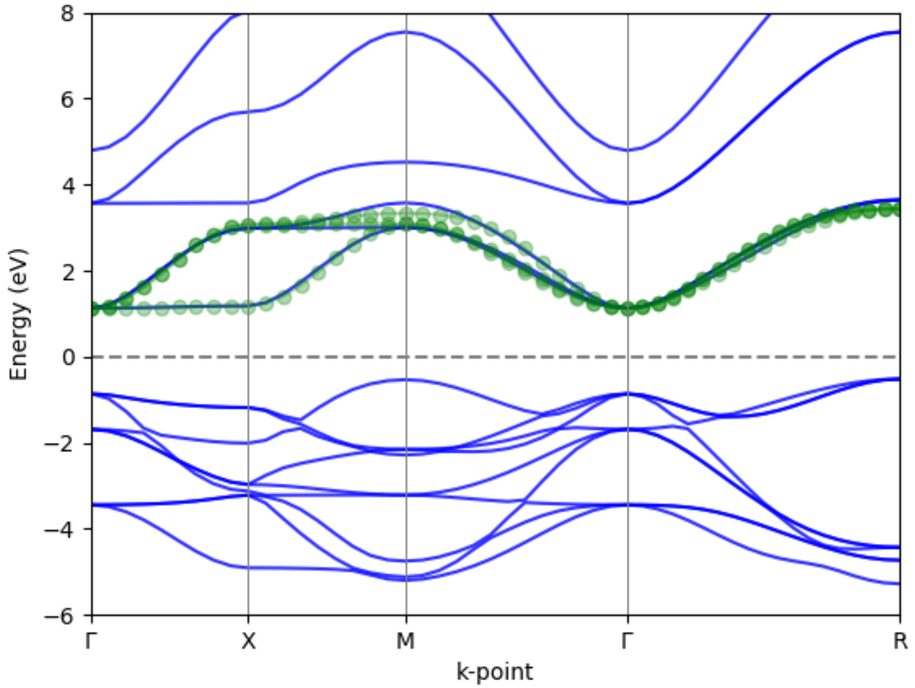


Example: BaTiO3

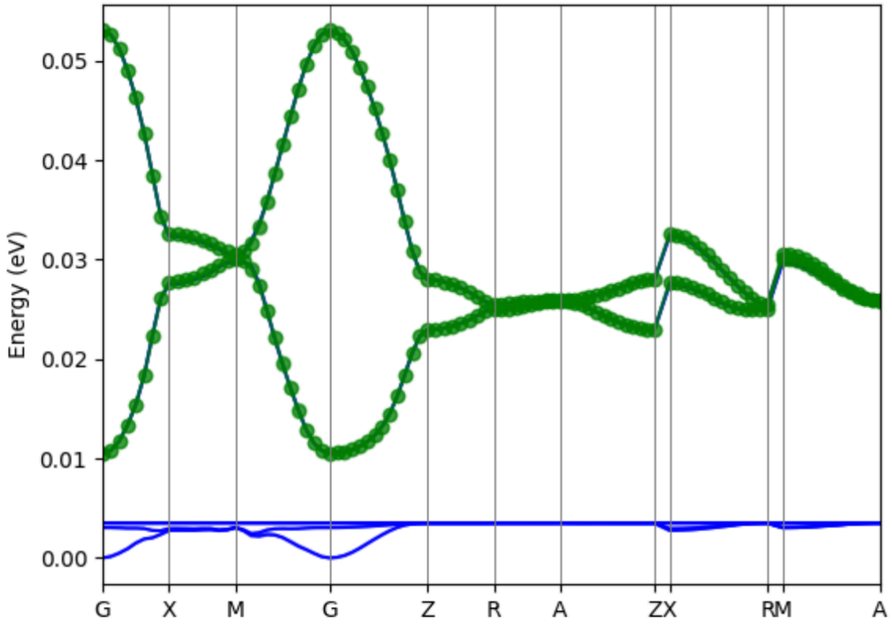
- Disentanglement made easy.
- dipole-dipole interaction.

With G.M. Rignanese, Ph. Ghosez

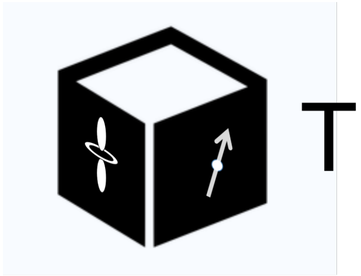
More than just Lattice Wannier functions



Electron Wannier function
(t2g bands of SrMnO3)



Magnon wannier function
(CoF2)

Updates on  TB2J

- A work flow for prediction of the magnetic ground state has been developed.

- [Ligand spin correction to exchange parameters with Wannierzation method] In some material, the spin magnetic moment of the ligand is non-negligible, and the interaction with metal magnetic moment affect the magnetic behaviour significantly. We developed a method to take the ligand contribution into account in the metal-metal J parameters.

More in Aldo’s talk

With Andres Mora, E.Bousquet, and A.Romero

Spin-phonon coupling from downfolding electron-phonon coupling parameters in TB2J

- $E = \sum_{ij} J_{ij} S_i S_j$

$G\Delta G\Delta$

Spin rotation perturbation

- $E = \sum_{ij} J_{ij} S_i S_j + \sum_{ijk} O_{ijk} S_i S_j \tau_k + E(\tau)$

$G\Delta G\Delta G\delta H_{\tau_k}$

Electron-phonon Perturbation

- Green's function + spin rotation perturbation + electron-phonon perturbation.

with S. Poncé, E.Bousquet, G-M. Rignanese, M.Verstraete

Using symmetrized Wannier function in TB2J

(Maximally localized) Wannier functions:

Spin up and down are not symmetric.

Does not preserve the crystal symmetry.

This can be problematic for using MLWF to represent spin-rotation perturbation

Wannier.jl:

Implementation of MLWF with

constraints on spin up/down symmetry

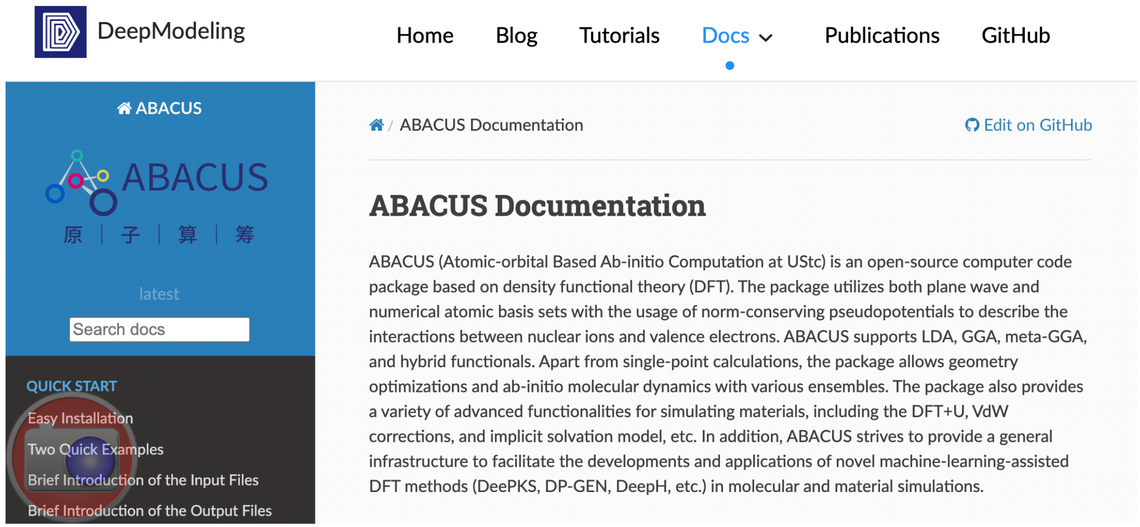
and Wannier centers.

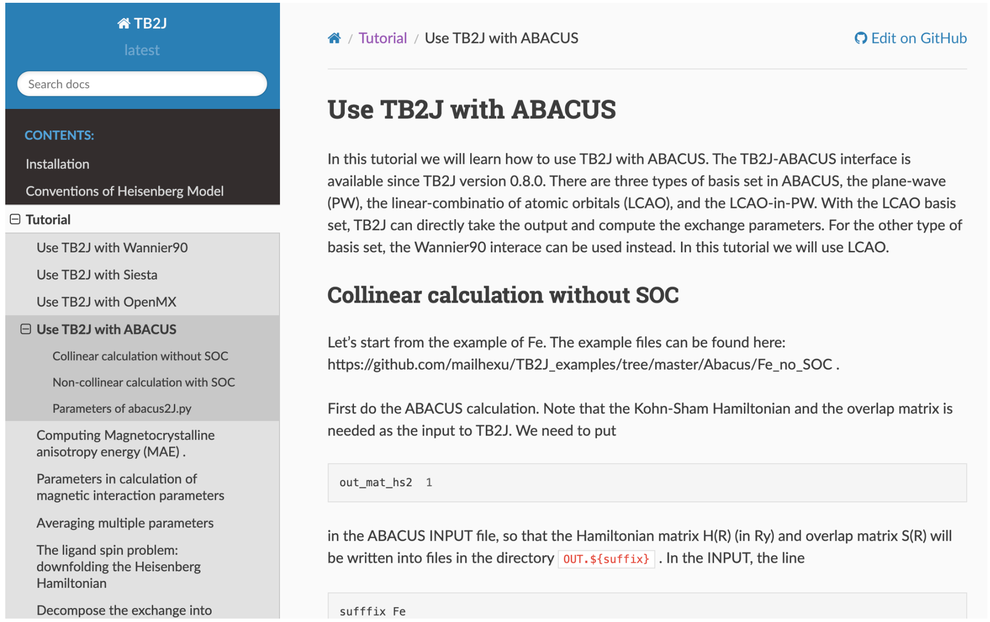
Testing of usage MLWF with various symmetry constraint.

Finding the best stategy of using Wannier functions in TB2J.

With M.Regout, M.Verstraete, JF.Qiao,G.Pizzi, D.Flaviano, M.Gilbertini

New interface to ABACUS



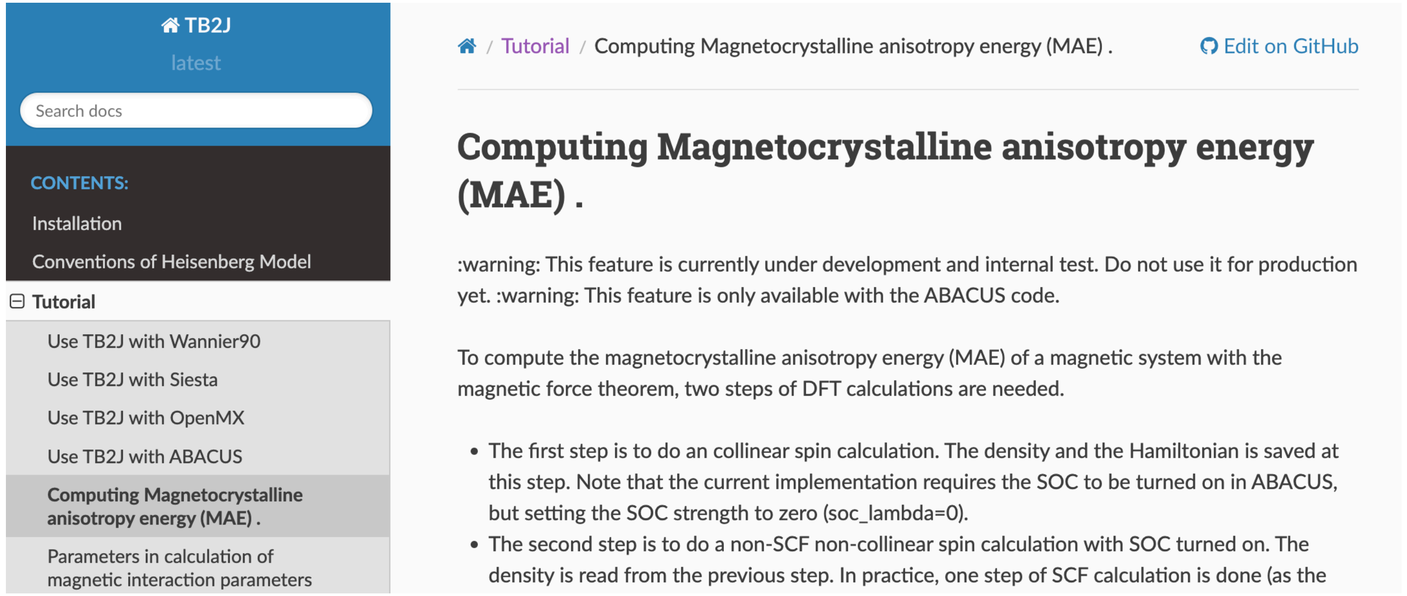


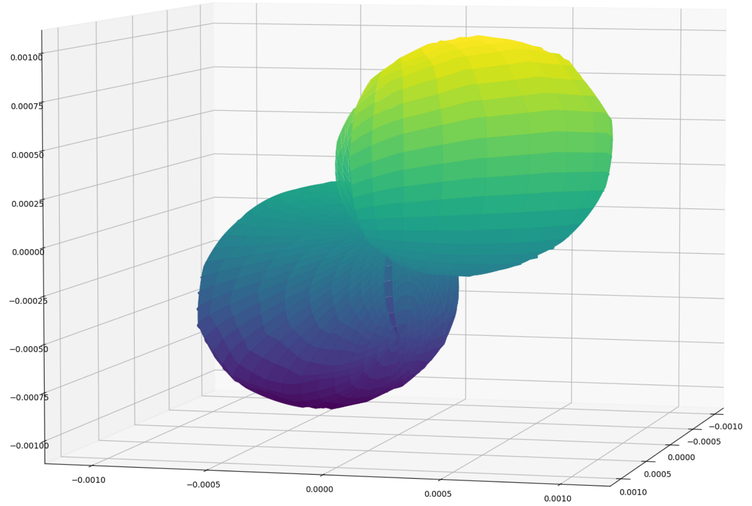
https://abacus.deepmodeling.com/en/latest/

https://tb2j.readthedocs.io/en/latest/src/abacus.html

In collaboration with Z.X. Shen and G.Jin from ABACUS group

Magnetocrystalline anisotropy energy (testing stage)





Implementation based on Magnetic force theorem (treating SOC as perturbation)