

Wannier90 v3.0 school, Virtual Edition 2020

Speaker: Arash Mostofi

25 March 2020 - Questions and answers session

- **What is the strategy to avoid introducing unnecessary bugs into the codes? When the programs become big, it will become hard to handle bugs.**
 - This of course becomes a bigger issue when moving to a model in which a larger community of developers contribute to the code as the scope for it to happen increases. We need to try to mitigate the risk. On one level, pull requests are automatically tested on the suite of tests using Travis CI and any test failure results in the pull request being blocked. This relies on the test suite having a very significant coverage of the code, which is something we all should continue to improve. As a second level, all pull requests are typically reviewed by one or more members of the Wannier Developers Group before merging into the main code. Bugs will, of course, still slip through, so we do need to continue thinking about how to improve this.
 - From Yusuke: The effort of going toward the library will help a lot I think. The code could be separated into a very stable core, and more experimental / actively developed satellite functionality.
- **The library mode is useful for e.g. EPW and AbInit; it's the most important thing that is missing and that can increase the number of contributors; great that it's happening.**
 - Thanks.
- **Is it possible to calculate the spin Hall conductivity using the wannier90 interfaced with VASP code?**
 - One note from one of the users: One can use the VASP interface with wannier 2.1. I am also not a VASP developer but I have done a lot of testing with VASP and constantly use VASP with wannier 2.1.
- **Do you have plans for introducing binary i/o such as netCDF? e.g. for amn, mmn and _hr.dat files**
 - This is not currently on the list of things to do, but if you think it's useful and important, then we'd be very happy to support its development if someone would like to lead it.
- **What is the bug-reporting mechanism at the moment? Is it mostly the mailing list?**
 - The mailing list is primarily intended for user queries about running the code. The github site is where we encourage bugs and code issues to be reported.

- **Is it possible to use the symmetry adapted WF in magnetic systems?**
 - Answer by Yusuke Nomura: unfortunately, it is not possible for the moment. It's more complex when having non-collinear spin, one needs to consider also the double group. for collinear magnetic states, I think you can make symmetry-adapted WFs separately for up and down spins (though I have never checked by myself, so please check when you try). For noncollinear magnetism, we can not apply symmetry-adapted mode.
- **What is the recommended procedure for generating maximally localized WFs in systems containing a lot of vacuum (2D systems, vdW crystals...)?**
 - Running a Gamma-point-only calculation to obtain an approximate set of WFs and WF centres to then seed the projection for a fully BZ-sampled calculation might help.
 - The SCDM method (talk and tutorial on this tomorrow) might also help with disentanglement in these cases.
 - From QuanSheng Wu: I just increase the kmesh along z direction more than 2
 - From Giovanni Pizzi: try setting the guiding_centres input parameter
- **General question: in the case of a unit cell with several equivalent atoms, can one enforce the spread of the Wannier functions sitting on the equivalent atoms to be the same along the minimization procedure (i.e., a sort of constrained minimization)?**
 - Answer from Yusuke Nomura: it is possible with symmetry-adapted mode, which puts symmetry constraint on the minimization.