

Tutorial on how to run the automated workflow to obtain interpolated bands using Wannier90, the SCDM method and the protocol described in the paper Automated High-throughput Wannierisation by Vitale *et al.*

All data, virtual machine, etc. can be found on the Materials Cloud Archive entry with doi <https://doi.org/10.24435/materialscloud:2019.0044/v2>

This document assumes that you have already properly obtained, installed and configured the virtual machine – if this not the case, please follow first the instructions in the file `README-virtual-machine.txt`

Acknowledgements

The virtual machine has been generated by modified versions of the MaX/MARVEL "Quantum Mobile" Virtual machine, whose original version can be found here:

<https://www.materialscloud.org/work/quantum-mobile>

This version is adapted to contain only the codes relevant to this project, and to adapt to the exact code versions used in the work [1].

For maximal reproducibility, we also attach the ansible roles that allow to rebuild from scratch the Virtual Machine, using the Ansible and Vagrant softwares.

This Virtual Machine reproduces the work of the following paper [1].
Please cite this work if you use the automated workflows presented here.

[1] Valerio Vitale, Giovanni Pizzi, Antimo Marrazzo, Jonathan R. Yates, Nicola Marzari, Arash A. Mostofi, Automated high-throughput Wannierisation, preprint: arXiv:1909.00433 (2019), <https://arxiv.org/abs/1909.00433>

Running a bands interpolation for CaO

1. Open the terminal (icon on the left bar, represented by a black screen with a `>` symbol inside) and type `workon aiida` to enter the virtual environment where AiiDA is installed.

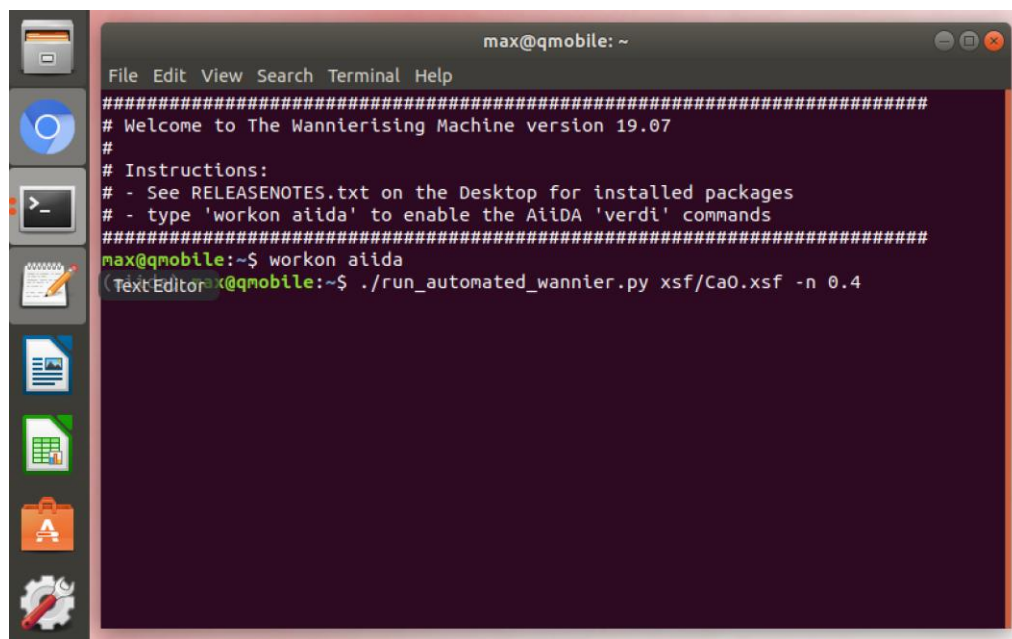
Then execute, in the home folder, the command

```
./run_automated_wannier.py xsf/CaO.xsf -n 0.4
```

to run the AiiDA workflows (using Quantum ESPRESSO and Wannier90, with the SCDM method) for CaO, using a linear density of k-points of 0.4 \AA^{-1} . This density, coarser than the one suggested in the paper, is used to speed up a bit the simulation, as you will be running with 2 CPUs on your workstation, and not on a supercomputer!

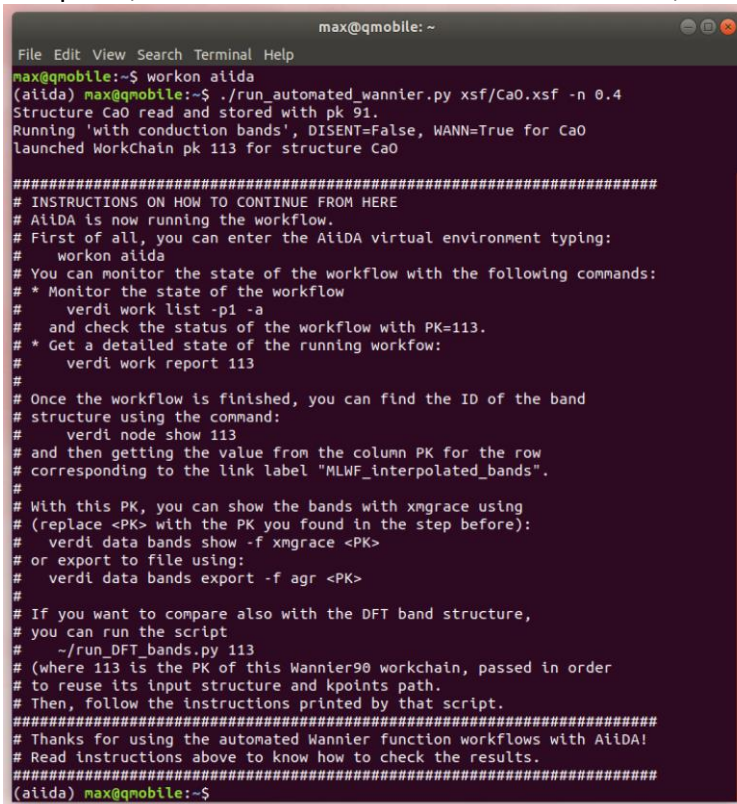
Notes:

- In the `xsf` subfolder you can also find all other materials used in the corresponding scientific paper.
- You can also run `./run_automated_wannier.py -h` to inspect other possible variables to change the behavior of the script (e.g. to choose a different density of k-points).



```
max@qmobile: ~
File Edit View Search Terminal Help
#####
# Welcome to The Wannierising Machine version 19.07
#
# Instructions:
# - See RELEASENOTES.txt on the Desktop for installed packages
# - type 'workon aiida' to enable the AiiDA 'verdi' commands
#####
max@qmobile:~$ workon aiida
(Text Editor) max@qmobile:~$ ./run_automated_wannier.py xsf/CaO.xsf -n 0.4
```

- When you run the script, it prints a long explanation of how to continue. The important information is the ID of the workflow (called WorkChain PK, in the screenshot below it is 113). Note that, depending on the performance of your computer, the workflow will take some time to run, at least a few minutes.



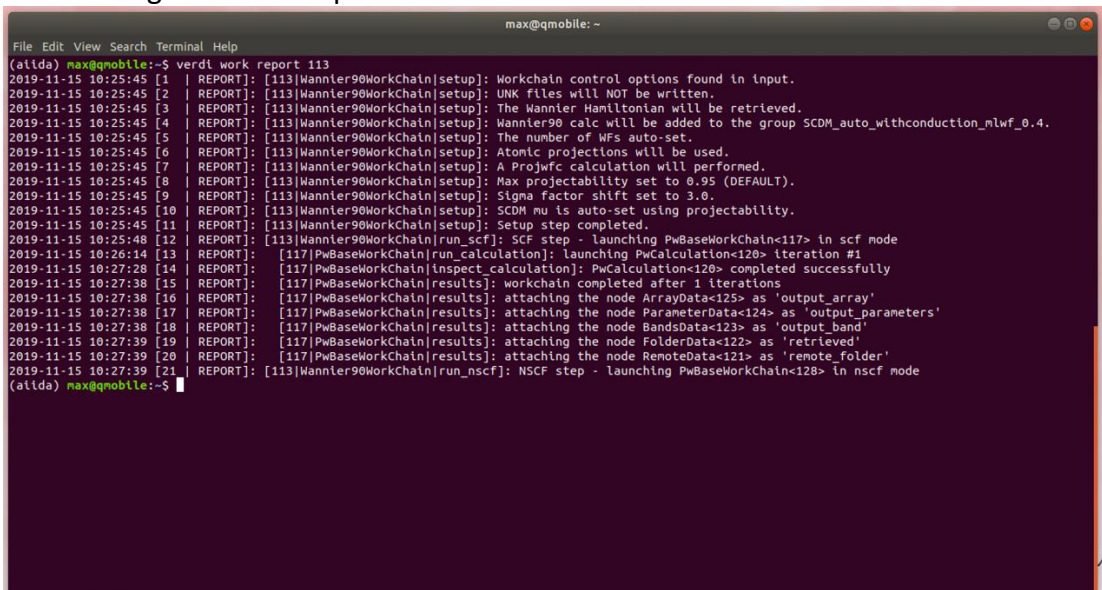
```

max@qmobile: ~
File Edit View Search Terminal Help
max@qmobile:~$ workon aiida
(aiida) max@qmobile:~$ ./run_automated_wannier.py xsf/Ca0.xsf -n 0.4
Structure Ca0 read and stored with pk 91.
Running 'with conduction bands', DISENT=False, WANN=True for Ca0
launched WorkChain pk 113 for structure Ca0

#####
# INSTRUCTIONS ON HOW TO CONTINUE FROM HERE
# AiIDA is now running the workflow.
# First of all, you can enter the AiIDA virtual environment typing:
#   workon aiida
# You can monitor the state of the workflow with the following commands:
# * Monitor the state of the workflow
#   verdi work list -p1 -a
# and check the status of the workflow with PK=113.
# * Get a detailed state of the running workflow:
#   verdi work report 113
#
# Once the workflow is finished, you can find the ID of the band
# structure using the command:
#   verdi node show 113
# and then getting the value from the column PK for the row
# corresponding to the link label "MLWF_interpolated_bands".
#
# With this PK, you can show the bands with xmgrace using
# (replace <PK> with the PK you found in the step before):
#   verdi data bands show -f xmgrace <PK>
# or export to file using:
#   verdi data bands export -f agr <PK>
#
# If you want to compare also with the DFT band structure,
# you can run the script
#   ~/run_DFT_bands.py 113
# (where 113 is the PK of this Wannier90 workchain, passed in order
# to reuse its input structure and kpoints path.
# Then, follow the instructions printed by that script.
#####
# Thanks for using the automated Wannier function workflows with AiIDA!
# Read instructions above to know how to check the results.
#####
(aiida) max@qmobile:~$

```

- You can check the list and status of recently run workflows with `verdi work list -p1 -a`
- If you want to inspect the workflow status, you can use the command `verdi work report 113` (replace 113 with the WorkChain PK obtained in the previous steps). The screenshot below, for instance, was taken while the workflow had completed the SCF step and was running the NSCF step.



```

max@qmobile: ~
File Edit View Search Terminal Help
(aiida) max@qmobile:~$ verdi work report 113
2019-11-15 10:25:45 [1] REPORT: [113|Wannier90WorkChain|setup]: Workchain control options found in input.
2019-11-15 10:25:45 [2] REPORT: [113|Wannier90WorkChain|setup]: UNK files will NOT be written.
2019-11-15 10:25:45 [3] REPORT: [113|Wannier90WorkChain|setup]: The Wannier Hamiltonian will be retrieved.
2019-11-15 10:25:45 [4] REPORT: [113|Wannier90WorkChain|setup]: Wannier90 calc will be added to the group SCDM_auto_withconduction_nlwf_0.4.
2019-11-15 10:25:45 [5] REPORT: [113|Wannier90WorkChain|setup]: The number of WFs auto-set.
2019-11-15 10:25:45 [6] REPORT: [113|Wannier90WorkChain|setup]: Atomic projections will be used.
2019-11-15 10:25:45 [7] REPORT: [113|Wannier90WorkChain|setup]: A ProjWfc calculation will be performed.
2019-11-15 10:25:45 [8] REPORT: [113|Wannier90WorkChain|setup]: Max projectability set to 0.95 (DEFAULT).
2019-11-15 10:25:45 [9] REPORT: [113|Wannier90WorkChain|setup]: Sigma factor shift set to 3.0.
2019-11-15 10:25:45 [10] REPORT: [113|Wannier90WorkChain|setup]: SCDM mu is auto-set using projectability.
2019-11-15 10:25:45 [11] REPORT: [113|Wannier90WorkChain|setup]: Setup step completed.
2019-11-15 10:25:48 [12] REPORT: [113|Wannier90WorkChain|run_scf]: SCF step - launching PwBaseWorkChain<117> in scf mode
2019-11-15 10:26:14 [13] REPORT: [117|PwBaseWorkChain|run_calculation]: launching PwCalculation<120> iteration #1
2019-11-15 10:27:28 [14] REPORT: [117|PwBaseWorkChain|inspect_calculation]: PwCalculation<120> completed successfully
2019-11-15 10:27:38 [15] REPORT: [117|PwBaseWorkChain|results]: workchain completed after 1 iterations
2019-11-15 10:27:38 [16] REPORT: [117|PwBaseWorkChain|results]: attaching the node ArrayData<125> as 'output_array'
2019-11-15 10:27:38 [17] REPORT: [117|PwBaseWorkChain|results]: attaching the node ParameterData<124> as 'output_parameters'
2019-11-15 10:27:38 [18] REPORT: [117|PwBaseWorkChain|results]: attaching the node BandsData<123> as 'output_band'
2019-11-15 10:27:39 [19] REPORT: [117|PwBaseWorkChain|results]: attaching the node FolderData<122> as 'retrieved'
2019-11-15 10:27:39 [20] REPORT: [117|PwBaseWorkChain|results]: attaching the node RemoteData<121> as 'remote_folder'
2019-11-15 10:27:39 [21] REPORT: [113|Wannier90WorkChain|run_nscf]: NSCF step - launching PwBaseWorkChain<128> in nscf mode
(aiida) max@qmobile:~$

```


- The report is also useful to go and inspect the independent calculations that were run by AiiDA. For instance, in the screenshot below, we identify the PK of the Quantum ESPRESSO pw.x calculation that run the SCF step (PK=120).

```

max@qmobile: ~
(aiida) max@qmobile:~$ verdi work report 113
2019-11-15 10:25:45 [1] REPORT: [113|Wannier90WorkChain|setup]: Workchain control options found in input.
2019-11-15 10:25:45 [2] REPORT: [113|Wannier90WorkChain|setup]: UNK files will NOT be written.
2019-11-15 10:25:45 [3] REPORT: [113|Wannier90WorkChain|setup]: The Wannier Hamiltonian will be retrieved.
2019-11-15 10:25:45 [4] REPORT: [113|Wannier90WorkChain|setup]: Wannier90 calc will be added to the group SCDM_auto_withconduction_mlwf_0.4.
2019-11-15 10:25:45 [5] REPORT: [113|Wannier90WorkChain|setup]: The number of WFs auto-set.
2019-11-15 10:25:45 [6] REPORT: [113|Wannier90WorkChain|setup]: Atomic projections will be used.
2019-11-15 10:25:45 [7] REPORT: [113|Wannier90WorkChain|setup]: A Projwfc calculation will be performed.
2019-11-15 10:25:45 [8] REPORT: [113|Wannier90WorkChain|setup]: Max projectability set to 0.95 (DEFAULT).
2019-11-15 10:25:45 [9] REPORT: [113|Wannier90WorkChain|setup]: Sigma factor shift set to 3.0.
2019-11-15 10:25:45 [10] REPORT: [113|Wannier90WorkChain|setup]: SCDM mu is auto-set using projectability.
2019-11-15 10:25:45 [11] REPORT: [113|Wannier90WorkChain|setup]: Setup step completed.
2019-11-15 10:25:48 [12] REPORT: [113|Wannier90WorkChain|run_scf]: SCF step - launching PwBaseWorkChain<117> in scf mode
2019-11-15 10:26:14 [13] REPORT: [117|PwBaseWorkChain|run_calculation]: launching PwCalculation<120> iteration #1
2019-11-15 10:27:28 [14] REPORT: [117|PwBaseWorkChain|inspect_calculation]: PwCalculation<120> completed successfully
2019-11-15 10:27:38 [15] REPORT: [117|PwBaseWorkChain|results]: workchain completed after 1 iterations
2019-11-15 10:27:38 [16] REPORT: [117|PwBaseWorkChain|results]: attaching the node ArrayData<125> as 'output_array'
2019-11-15 10:27:38 [17] REPORT: [117|PwBaseWorkChain|results]: attaching the node ParameterData<124> as 'output_parameters'
2019-11-15 10:27:38 [18] REPORT: [117|PwBaseWorkChain|results]: attaching the node BandsData<123> as 'output_band'
2019-11-15 10:27:39 [19] REPORT: [117|PwBaseWorkChain|results]: attaching the node FolderData<122> as 'retrieved'
2019-11-15 10:27:39 [20] REPORT: [117|PwBaseWorkChain|results]: attaching the node RemoteData<121> as 'remote_folder'
2019-11-15 10:27:39 [21] REPORT: [113|Wannier90WorkChain|run_nscf]: NSCF step - launching PwBaseWorkChain<128> in nscf mode
(aiida) max@qmobile:~$

```

- With this PK, we can check the results of the Quantum ESPRESSO calculation itself. AiiDA provides different ways of inspecting the results (raw and parsed). Here we show how to access the raw results, since they are most useful for users not experienced with AiiDA.

In particular (see screenshot below), you can open a terminal directly in the folder where the simulation run with the command `verdi calculation gotocomputer 120` (replace 120 with the PK of the PwCalculation). As shown below, you will find the various files (for instance, `aiida.in` is the pw.x input file, and `aiida.out` is the pw.x output file).

```

max@qmobile: ~/aiida_run/fe/45/324f-d859-481e-95cd-82743c4beb11
(aiida) max@qmobile:~$ clear
(aiida) max@qmobile:~$ verdi work report 113
2019-11-15 10:25:45 [1] REPORT: [113|Wannier90WorkChain|setup]: Workchain control options found in input.
2019-11-15 10:25:45 [2] REPORT: [113|Wannier90WorkChain|setup]: UNK files will NOT be written.
2019-11-15 10:25:45 [3] REPORT: [113|Wannier90WorkChain|setup]: The Wannier Hamiltonian will be retrieved.
2019-11-15 10:25:45 [4] REPORT: [113|Wannier90WorkChain|setup]: Wannier90 calc will be added to the group SCDM_auto_withconduction_mlwf_0.4.
2019-11-15 10:25:45 [5] REPORT: [113|Wannier90WorkChain|setup]: The number of WFs auto-set.
2019-11-15 10:25:45 [6] REPORT: [113|Wannier90WorkChain|setup]: Atomic projections will be used.
2019-11-15 10:25:45 [7] REPORT: [113|Wannier90WorkChain|setup]: A Projwfc calculation will be performed.
2019-11-15 10:25:45 [8] REPORT: [113|Wannier90WorkChain|setup]: Max projectability set to 0.95 (DEFAULT).
2019-11-15 10:25:45 [9] REPORT: [113|Wannier90WorkChain|setup]: Sigma factor shift set to 3.0.
2019-11-15 10:25:45 [10] REPORT: [113|Wannier90WorkChain|setup]: SCDM mu is auto-set using projectability.
2019-11-15 10:25:45 [11] REPORT: [113|Wannier90WorkChain|setup]: Setup step completed.
2019-11-15 10:25:48 [12] REPORT: [113|Wannier90WorkChain|run_scf]: SCF step - launching PwBaseWorkChain<117> in scf mode
2019-11-15 10:26:14 [13] REPORT: [117|PwBaseWorkChain|run_calculation]: launching PwCalculation<120> iteration #1
2019-11-15 10:27:28 [14] REPORT: [117|PwBaseWorkChain|inspect_calculation]: PwCalculation<120> completed successfully
2019-11-15 10:27:38 [15] REPORT: [117|PwBaseWorkChain|results]: workchain completed after 1 iterations
2019-11-15 10:27:38 [16] REPORT: [117|PwBaseWorkChain|results]: attaching the node ArrayData<125> as 'output_array'
2019-11-15 10:27:38 [17] REPORT: [117|PwBaseWorkChain|results]: attaching the node ParameterData<124> as 'output_parameters'
2019-11-15 10:27:38 [18] REPORT: [117|PwBaseWorkChain|results]: attaching the node BandsData<123> as 'output_band'
2019-11-15 10:27:39 [19] REPORT: [117|PwBaseWorkChain|results]: attaching the node FolderData<122> as 'retrieved'
2019-11-15 10:27:39 [20] REPORT: [117|PwBaseWorkChain|results]: attaching the node RemoteData<121> as 'remote_folder'
2019-11-15 10:27:39 [21] REPORT: [113|Wannier90WorkChain|run_nscf]: NSCF step - launching PwBaseWorkChain<128> in nscf mode
(aiida) max@qmobile:~$ verdi calculation gotocomputer 120
Loading environment...
Going to the remote folder...
#####
# Welcome to The Wannier90 Machine version 19.07
#
# Instructions:
# - See RELEASNOTES.txt on the Desktop for installed packages
# - type 'workon aiida' to enable the AiiDA 'verdi' commands
#####
max@qmobile:~/aiida_run/fe/45/324f-d859-481e-95cd-82743c4beb11$ ls
aiida.in  aiida.out  aiidasubmit.sh  out  pseudo_scheduler-stderr.txt  scheduler-stdout.txt
max@qmobile:~/aiida_run/fe/45/324f-d859-481e-95cd-82743c4beb11$ head aiida.out
Program PWSCF v.6.3MaX starts on 15Nov2019 at 11:26:25

This program is part of the open-source Quantum ESPRESSO suite
for quantum simulation of materials; please cite
"P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502 (2009);
"P. Giannozzi et al., J. Phys.:Condens. Matter 29 465901 (2017);
URL http://www.quantum-espresso.org",
in publications or presentations arising from this work. More details at
http://www.quantum-espresso.org/quote
max@qmobile:~/aiida_run/fe/45/324f-d859-481e-95cd-82743c4beb11$

```

- Once you have finished inspecting the files, you can type `exit` (only once) to go back to the terminal with the AiIDA virtual environment.
- When the workflow completes, `verdi work list -p1 -a` will list all workflows and subworkflows as `Finished`.

Additionally, the last line of `verdi work report 113` will state that the `Wannier90WorkChain` successfully completed.

In the report, you will also find the PKs of all calculations that were run. In the following screenshot, for instance, these are:

- `PwCalculation` (Quantum ESPRESSO `pw.x`, SCF step): 120
- `PwCalculation` (Quantum ESPRESSO `pw.x`, NSCF step): 131
- `ProjwfcCalculation` (Quantum ESPRESSO `projwfc.x`): 137
- `Wannier90Calculation` (preprocess mode): 153
- `Pw2wannier90Calculation` (Quantum ESPRESSO `pw2wannier90.x`): 159
- `Wannier90Calculation` (main run): 166

As before, you can use the command `verdi calculation gotocomputer PK` (replacing PK with the correct PK) to go to the folder where the simulation has run and inspect the raw inputs and outputs from Quantum ESPRESSO or `wannier90`). Additionally, also the PK of the final interpolated band structure is reported: 169

```

max@qmobile: ~
File Edit View Search Terminal Help
(aiida) max@qmobile:~$ verdi work list -p1 -a
-----
PK      Creation      State      Sealed      ProcessLabel
-----
93      23m ago         Finished   True        seekpath_structure_analysis
113     23m ago         Finished   True        Wannier90WorkChain
117     23m ago         Finished   True        PwBaseWorkChain
128     22m ago         Finished   True        PwBaseWorkChain
144     17m ago         Finished   True        set_auto_nunwann
147     17m ago         Finished   True        set_mu_and_sigma_from_projections
150     17m ago         Finished   True        from_seekpath_to_wannier
163     15m ago         Finished   True        from_seekpath_to_wannier
(aiida) max@qmobile:~$ verdi work report 113
2019-11-15 10:25:45 [1] REPORT: [113]Wannier90WorkChain[setup]: Workchain control options found in input.
2019-11-15 10:25:45 [2] REPORT: [113]Wannier90WorkChain[setup]: UNK files will NOT be written.
2019-11-15 10:25:45 [3] REPORT: [113]Wannier90WorkChain[setup]: The Wannier Hamiltonian will be retrieved.
2019-11-15 10:25:45 [4] REPORT: [113]Wannier90WorkChain[setup]: Wannier90 calc will be added to the group 'SCDM_auto_withconduction_nlwf_0.4'.
2019-11-15 10:25:45 [5] REPORT: [113]Wannier90WorkChain[setup]: The number of WFs auto-set.
2019-11-15 10:25:45 [6] REPORT: [113]Wannier90WorkChain[setup]: Atomic projections will be used.
2019-11-15 10:25:45 [7] REPORT: [113]Wannier90WorkChain[setup]: A Projwfc calculation will be performed.
2019-11-15 10:25:45 [8] REPORT: [113]Wannier90WorkChain[setup]: Max projectability set to 0.95 (DEFAULT).
2019-11-15 10:25:45 [9] REPORT: [113]Wannier90WorkChain[setup]: Sigma factor shift set to 3.0.
2019-11-15 10:25:45 [10] REPORT: [113]Wannier90WorkChain[setup]: SCDM mu is auto-set using projectability.
2019-11-15 10:25:45 [11] REPORT: [113]Wannier90WorkChain[setup]: Setup step completed.
2019-11-15 10:25:48 [12] REPORT: [113]Wannier90WorkChain[run_scf]: SCF step - launching PwBaseWorkChain-117 in scf mode
2019-11-15 10:26:14 [13] REPORT: [117]PwBaseWorkChain[run_calculation]: launching PwCalculation-120 iteration #1
2019-11-15 10:27:28 [14] REPORT: [117]PwBaseWorkChain[inspect calculation]: PwCalculation-120 completed successfully
2019-11-15 10:27:38 [15] REPORT: [117]PwBaseWorkChain[results]: workchain completed after 1 iterations
2019-11-15 10:27:38 [16] REPORT: [117]PwBaseWorkChain[results]: attaching the node ArrayData-125 as 'output_array'
2019-11-15 10:27:38 [17] REPORT: [117]PwBaseWorkChain[results]: attaching the node ParameterData-124 as 'output_parameters'
2019-11-15 10:27:38 [18] REPORT: [117]PwBaseWorkChain[results]: attaching the node BandsData-123 as 'output_band'
2019-11-15 10:27:39 [19] REPORT: [117]PwBaseWorkChain[results]: attaching the node FolderData-122 as 'retrieved'
2019-11-15 10:27:39 [20] REPORT: [117]PwBaseWorkChain[results]: attaching the node RemoteData-121 as 'remote_folder'
2019-11-15 10:27:39 [21] REPORT: [113]Wannier90WorkChain[run_nscf]: NSCF step - launching PwBaseWorkChain-128 in nscf mode
2019-11-15 10:28:03 [22] REPORT: [128]PwBaseWorkChain[run_calculation]: launching PwCalculation-131 iteration #1
2019-11-15 10:31:28 [23] REPORT: [128]PwBaseWorkChain[inspect calculation]: PwCalculation-131 completed successfully
2019-11-15 10:31:39 [24] REPORT: [128]PwBaseWorkChain[results]: workchain completed after 1 iterations
2019-11-15 10:31:39 [25] REPORT: [128]PwBaseWorkChain[results]: attaching the node ArrayData-136 as 'output_array'
2019-11-15 10:31:39 [26] REPORT: [128]PwBaseWorkChain[results]: attaching the node ParameterData-135 as 'output_parameters'
2019-11-15 10:31:39 [27] REPORT: [128]PwBaseWorkChain[results]: attaching the node BandsData-134 as 'output_band'
2019-11-15 10:31:39 [28] REPORT: [128]PwBaseWorkChain[results]: attaching the node FolderData-133 as 'retrieved'
2019-11-15 10:31:39 [29] REPORT: [128]PwBaseWorkChain[results]: attaching the node RemoteData-132 as 'remote_folder'
2019-11-15 10:31:44 [30] REPORT: [113]Wannier90WorkChain[run_projwfc]: PROJWFC step - launching ProjwfcCalculation-137.
2019-11-15 10:32:26 [31] REPORT: [113]Wannier90WorkChain[run_wannier90_pp]: MLWF PP step - launching Wannier90 Calculation <153> in pp mode
2019-11-15 10:32:53 [32] REPORT: [113]Wannier90WorkChain[run_pw2wannier90]: Pw2wannier90 step - launching Pw2Wannier90 Calculation <159>
2019-11-15 10:34:14 [33] REPORT: [113]Wannier90WorkChain[run_wannier90]: MLWF step - launching Wannier90 Calculation <166>
2019-11-15 10:35:24 [34] REPORT: [113]Wannier90WorkChain[results]: Final step, preparing outputs
2019-11-15 10:35:24 [35] REPORT: [113]Wannier90WorkChain[results]: Interpolated bands pk: 169
2019-11-15 10:35:24 [36] REPORT: [113]Wannier90WorkChain[results]: Wannier90WorkChain successfully completed.
(aiida) max@qmobile:~$

```

- Equivalently, the PK of the interpolated band structure can be obtained by inspecting the output nodes of the initial workflow that we submitted (it was PK=113 in our example). This can be done by running the command `verdi node show 113` and checking the PK of the output node with link label `MLWF_interpolated_bands`. Indeed, as shown in the screenshot below, the PK

is 169, the same we obtained from the output of `verdi work report 113`.

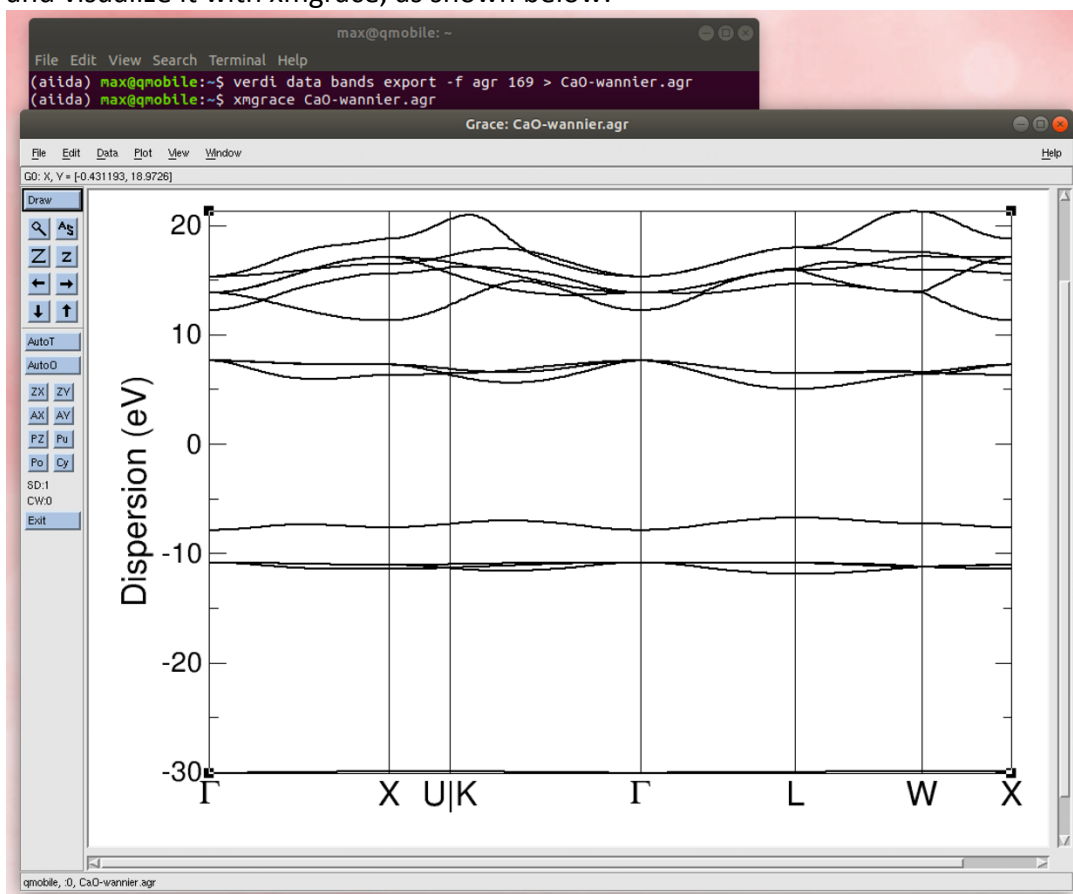
```

max@qmobile: ~
File Edit View Search Terminal Help
(aiida) max@qmobile:~$ verdi node show 113 | tail -n 28
##### OUTPUTS:
Link label                                     PK  Type
-----
CALL                                           144  WorkCalculation
CALL                                           128  WorkCalculation
CREATE                                         127  ParameterData
CREATE                                         114  ParameterData
mlwf_output_parameters                        170  ParameterData
overlap_matrices_local_folder                161  FolderData
CREATE                                         126  ParameterData
nscf_output_parameters                       135  ParameterData
CALL                                           117  WorkCalculation
CREATE                                         115  Bool
CREATE                                         116  Int
CALL                                           166  Wannier90Calculation
CREATE                                         146  ParameterData
CALL                                           137  ProjwfcCalculation
CALL                                           150  WorkCalculation
overlap_matrices_remote_folder               160  RemoteData
CALL                                           159  Pw2wannier90Calculation
CALL                                           153  Wannier90Calculation
scf output parameters                       124  ParameterData
MLWF interpolated bands                      169  BandsData
CALL                                           147  WorkCalculation
CALL                                           163  WorkCalculation
##### LOGS:
There are 20 log messages for this calculation
Run 'verdi work report 113' to see them
(aiida) max@qmobile:~$

```

10. Finally, you can export the band structure (e.g. in `xmgrace .agr` format) with the command

`verdi data bgbands export -f -agr 169 > CaO-wannier.agr`
and visualize it with `xmgrace`, as shown below:



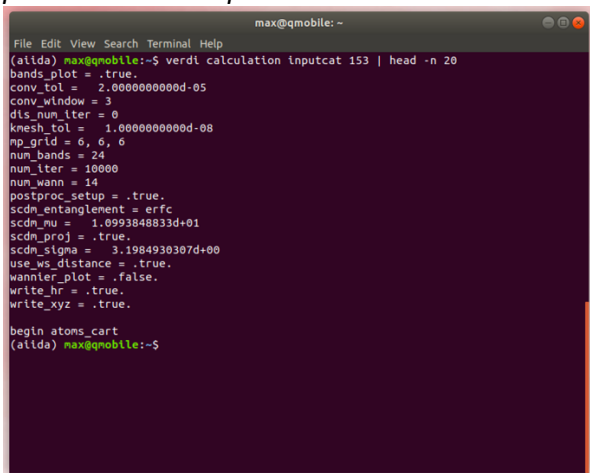
Extract the SCDM parameters

We now discuss how to extract the SCDM μ and σ parameters from the automatic workflow, and how to obtain them in general also without the AiiDA workflows described in the paper.

1. To obtain the parameters used in the run, use the command `verdi calculation inputcat 166` (where 166 is the PK of the Wannier90 calculation, obtained above). Among the parameters you will find the values, in this case (see also screenshot below)

```
scdm_mu = 1.0993848833d+01
scdm_sigma = 3.1984930307d+00
```

An important note: in more recent versions of Quantum ESPRESSO and Wannier90, these values are not present anymore in the Wannier90 input, but directly in the pw2wannier90 input.



```
max@qmobile: ~
File Edit View Search Terminal Help
(aiida) max@qmobile:~$ verdi calculation inputcat 153 | head -n 20
bands_plot = .true.
conv_tol = 2.0000000000d-05
conv_window = 3
dis_num_iter = 0
kmesh_tol = 1.0000000000d-08
mp_grid = 6, 6, 6
num_bands = 24
num_iter = 10000
num_wann = 14
postproc_setup = .true.
scdm_entanglement = erfc
scdm_mu = 1.0993848833d+01
scdm_proj = .true.
scdm_sigma = 3.1984930307d+00
use_ws_distance = .true.
wannier_plot = .false.
write_hr = .true.
write_xyz = .true.

begin atoms_cart
(aiida) max@qmobile:~$
```

2. If instead you want to compute the values yourself, without using the automated workflow, you will need to reproduce the fit of Fig. 8 of the Vitale *et al.* paper. To this aim, we describe below the algorithm to be followed:
 - a. Get the squared modulus of the projection of a given wavefunction (n , \mathbf{k}) of each of the atomic orbitals defined in the pseudopotential files. This is computed by the `projwfc.x` code. If you want to inspect the output, you can see it with `verdi calculation gotocomputer 137` in our example.
 - b. Sum these components for each given (n , \mathbf{k}) for all orbitals, to obtain the projectability of the band (n , \mathbf{k}).
 - c. Plot these projectability values (on the y axis) vs. the energy of the corresponding band E_{nk} , obtaining a plot similar to Fig. 8 of the paper. You might want to exclude all n values associated to excluded bands, if you are excluding bands in the Wannier90 calculation.
 - d. Fit the resulting points with the following function:
$$f(x) = 0.5 \operatorname{erfc}((x - \mu_{\text{fit}})/\sigma_{\text{fit}})$$
 - e. Obtain the SCDM parameters as $\mu_{\text{SCDM}} = \mu_{\text{fit}} - 3\sigma_{\text{fit}}$, $\sigma_{\text{SCDM}} = \sigma_{\text{fit}}$
3. *Note:* this algorithm is implemented in the AiiDA parser (for the extraction of the data from the output of `projwfc.x`) and in the function `set_mu_and_sigma_from_projections` at the bottom of the workflow file that you can find in the virtual machine at the path:

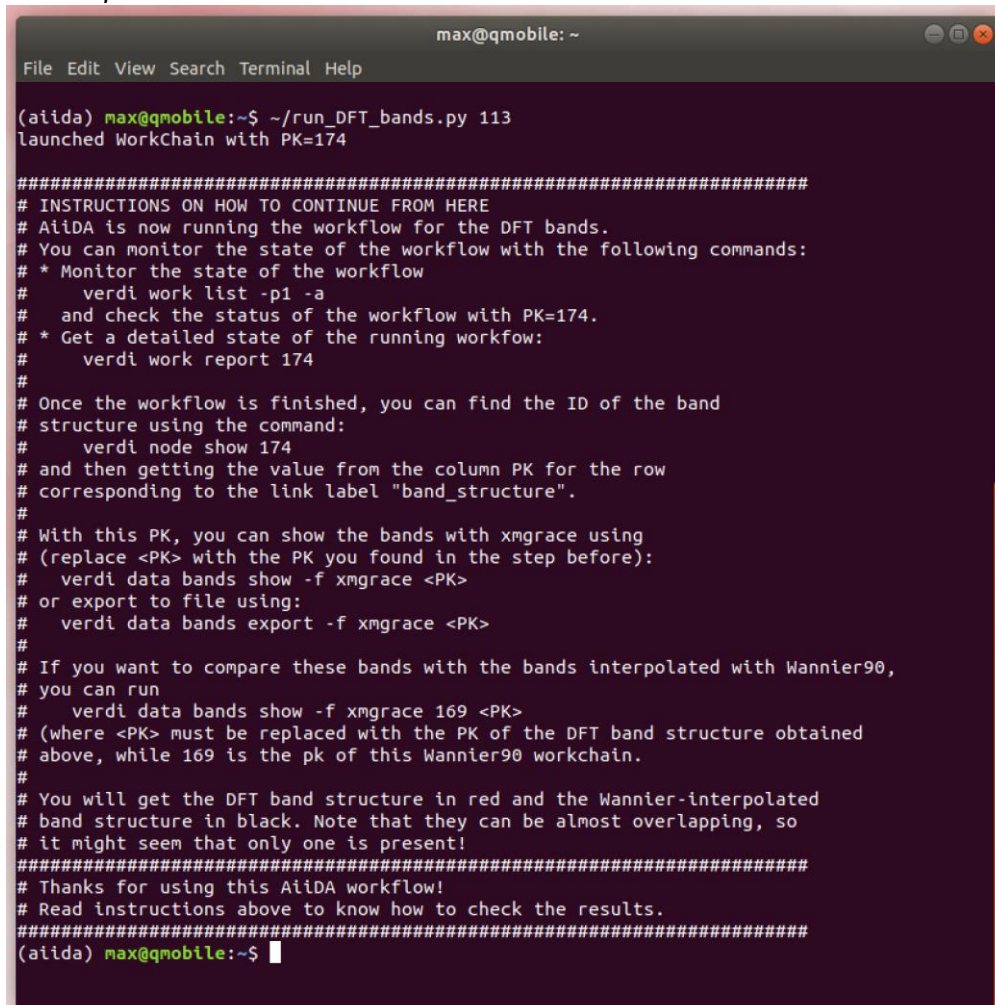
```
~/codes/aiida-wannier90-theosworkflows/aiida_wannier90_theosworkflows/workflows
```

Compare the interpolated bands with the DFT bands

We now discuss how to run also the bands with DFT and compare them with the interpolated bands.

1. Run the script `~/run_DFT_bands.py 113` to start a workflow computing the bands using DFT on the same crystal structure. As usual, replace 113 with the Wannier WorkChain PK obtained at the beginning.

Note that the Wannier90 WorkChain needs to have completed before you can run this script.



```
max@qmobile: ~  
File Edit View Search Terminal Help  
  
(aiida) max@qmobile:~$ ~/run_DFT_bands.py 113  
Launched WorkChain with PK=174  
  
#####  
# INSTRUCTIONS ON HOW TO CONTINUE FROM HERE  
# AiIDA is now running the workflow for the DFT bands.  
# You can monitor the state of the workflow with the following commands:  
# * Monitor the state of the workflow  
#   verdi work list -p1 -a  
#   and check the status of the workflow with PK=174.  
# * Get a detailed state of the running workflow:  
#   verdi work report 174  
#  
# Once the workflow is finished, you can find the ID of the band  
# structure using the command:  
#   verdi node show 174  
# and then getting the value from the column PK for the row  
# corresponding to the link label "band_structure".  
#  
# With this PK, you can show the bands with xmgrace using  
# (replace <PK> with the PK you found in the step before):  
#   verdi data bands show -f xmgrace <PK>  
# or export to file using:  
#   verdi data bands export -f xmgrace <PK>  
#  
# If you want to compare these bands with the bands interpolated with Wannier90,  
# you can run  
#   verdi data bands show -f xmgrace 169 <PK>  
# (where <PK> must be replaced with the PK of the DFT band structure obtained  
# above, while 169 is the pk of this Wannier90 workchain.  
#  
# You will get the DFT band structure in red and the Wannier-interpolated  
# band structure in black. Note that they can be almost overlapping, so  
# it might seem that only one is present!  
#####  
# Thanks for using this AiIDA workflow!  
# Read instructions above to know how to check the results.  
#####  
(aiida) max@qmobile:~$
```

2. The output of the previous script instructs on how to plot the bands. In summary, you will have launched a new WorkChain (in this case for DFT bands, and in the example above with PK=174). You can use (as before) the commands `verdi work list -p1 -a` to check the workflow completion and `verdi work report 174` to see the report of the workflow.

We show below the output of the two commands when the workflow has completed. In particular, in the output of the report, you can find (numbers refer to our specific example shown below):

- a. PwCalculation (Quantum ESPRESSO pw.x, SCF step): PK=191
- b. PwCalculation (Quantum ESPRESSO pw.x, NSCF step): PK=201

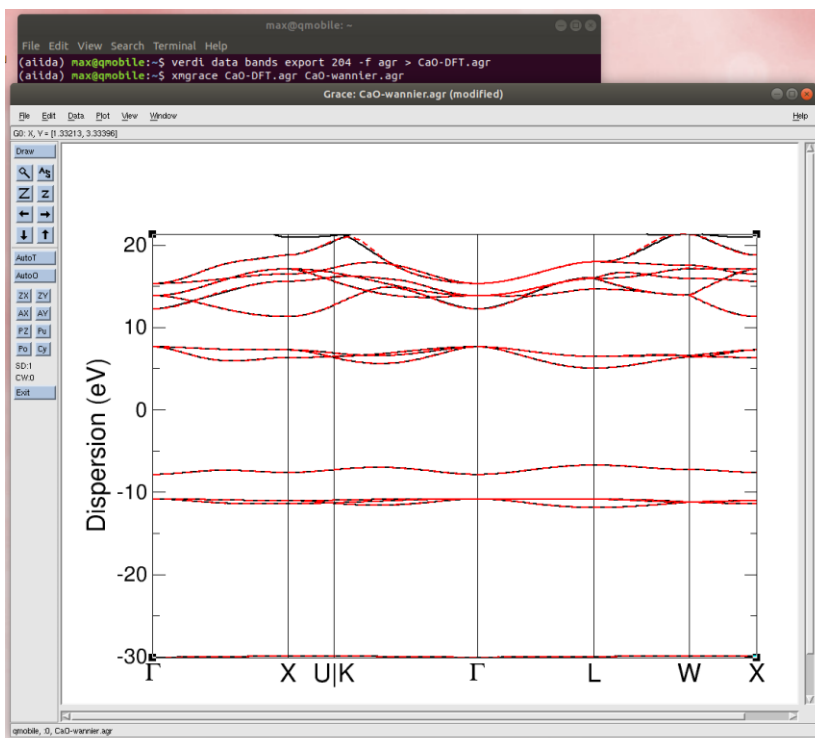
In addition, we can get from the last line the PK of the output DFT bands (link label: `band_structure`). In our example: PK=204


```

max@qmobile: ~
File Edit View Search Terminal Help
(alida) max@qmobile:~$ verdi work list -p1 -a
-----
PK      Creation      State      Sealed      ProcessLabel
-----
93      1h ago             Finished   True        seekpath_structure_analysis
113     1h ago             Finished   True        wannierizeWorkChain
117     1h ago             Finished   True        PwBaseWorkChain
128     1h ago             Finished   True        PwBaseWorkChain
144     1h ago             Finished   True        set_auto_numwann
147     1h ago             Finished   True        set_mu_and_signs_from_projections
150     1h ago             Finished   True        from_seekpath_to_wannier
163     1h ago             Finished   True        from_seekpath_to_wannier
174     12m ago            Finished   True        customPwBandStructureWorkChain
183     11n ago            Finished   True        PwBandsWorkChain
188     11n ago            Finished   True        PwBaseWorkChain
198     9m ago             Finished   True        PwBaseWorkChain
(alida) max@qmobile:~$ verdi work report 174
2019-11-15 12:04:59 [37] REPORT: [174]CustomPwBandStructureWorkChain[setup_protocol]: running the workchain in the "standard" protocol
2019-11-15 12:05:14 [38] REPORT: [174]CustomPwBandStructureWorkChain[run_bands]: launching PwBandsWorkChain<183>
2019-11-15 12:05:29 [39] REPORT: [183]PwBandsWorkChain[only_scf]: only_scf specified to True
2019-11-15 12:05:34 [40] REPORT: [183]PwBandsWorkChain[run_scf]: DEBUG - SCF STEP
2019-11-15 12:05:34 [41] REPORT: [183]PwBandsWorkChain[run_scf]: launching PwBaseWorkChain<188> in scf mode
2019-11-15 12:05:59 [42] REPORT: [188]PwBaseWorkChain[run_calculation]: launching PwCalculation<191> iteration #1
2019-11-15 12:06:54 [43] REPORT: [188]PwBaseWorkChain[inspect_calculation]: PwCalculation<191> completed successfully
2019-11-15 12:07:04 [45] REPORT: [188]PwBaseWorkChain[results]: workchain completed after 1 iterations
2019-11-15 12:07:04 [46] REPORT: [188]PwBaseWorkChain[results]: attaching the node ArrayData<196> as 'output_array'
2019-11-15 12:07:04 [47] REPORT: [188]PwBaseWorkChain[results]: attaching the node ParameterData<195> as 'output_parameters'
2019-11-15 12:07:04 [48] REPORT: [188]PwBaseWorkChain[results]: attaching the node BandsData<194> as 'output_band'
2019-11-15 12:07:04 [49] REPORT: [188]PwBaseWorkChain[results]: attaching the node FolderData<193> as 'retrieved'
2019-11-15 12:07:04 [50] REPORT: [188]PwBaseWorkChain[results]: attaching the node RemoteData<192> as 'remote_folder'
2019-11-15 12:07:09 [51] REPORT: [183]PwBandsWorkChain[run_bands]: launching PwBaseWorkChain<198> in bands mode
2019-11-15 12:07:34 [52] REPORT: [198]PwBaseWorkChain[run_calculation]: launching PwCalculation<201> iteration #1
2019-11-15 12:14:25 [53] REPORT: [198]PwBaseWorkChain[inspect_calculation]: PwCalculation<201> completed successfully
2019-11-15 12:14:35 [54] REPORT: [198]PwBaseWorkChain[results]: workchain completed after 1 iterations
2019-11-15 12:14:35 [55] REPORT: [198]PwBaseWorkChain[results]: attaching the node ArrayData<206> as 'output_array'
2019-11-15 12:14:35 [56] REPORT: [198]PwBaseWorkChain[results]: attaching the node ParameterData<205> as 'output_parameters'
2019-11-15 12:14:35 [57] REPORT: [198]PwBaseWorkChain[results]: attaching the node BandsData<204> as 'output_band'
2019-11-15 12:14:35 [58] REPORT: [198]PwBaseWorkChain[results]: attaching the node FolderData<203> as 'retrieved'
2019-11-15 12:14:35 [59] REPORT: [198]PwBaseWorkChain[results]: attaching the node RemoteData<202> as 'remote_folder'
2019-11-15 12:14:39 [60] REPORT: [183]PwBandsWorkChain[results]: workchain successfully completed
2019-11-15 12:14:39 [61] REPORT: [174]CustomPwBandStructureWorkChain[run_results]: workchain successfully completed
2019-11-15 12:14:39 [62] REPORT: [174]CustomPwBandStructureWorkChain[run_results]: attaching ParameterData<195> as an output node with label 'scf_parameters'
2019-11-15 12:14:39 [63] REPORT: [174]CustomPwBandStructureWorkChain[run_results]: attaching ParameterData<205> as an output node with label 'band_parameters'
2019-11-15 12:14:40 [64] REPORT: [174]CustomPwBandStructureWorkChain[run_results]: attaching BandsData<204> as an output node with label 'band_structure'
(alida) max@qmobile:~$

```

3. We can now export the bands with
`verdi data bands export 204 -f agr > CaO-DFT.agr`
 You can now plot both band structures overlapped using, for instance, xmgrace.
 (They both use the same k-points path computed by the seekpath¹ code.)
 You can run this with `xmgrace CaO-DFT.agr CaO-wannier.agr`
Note: in the plot below we have then changed the color of the Wannier-interpolated bands to use red-dashed thicker lines, leaving the DFT bands as black (the default is to use black lines for the first file specified, i.e., the DFT bands; and random colors – one per band – for the second file, i.e., the Wannier bands).



¹ <https://materialscloud.org/tools/seekpath/>