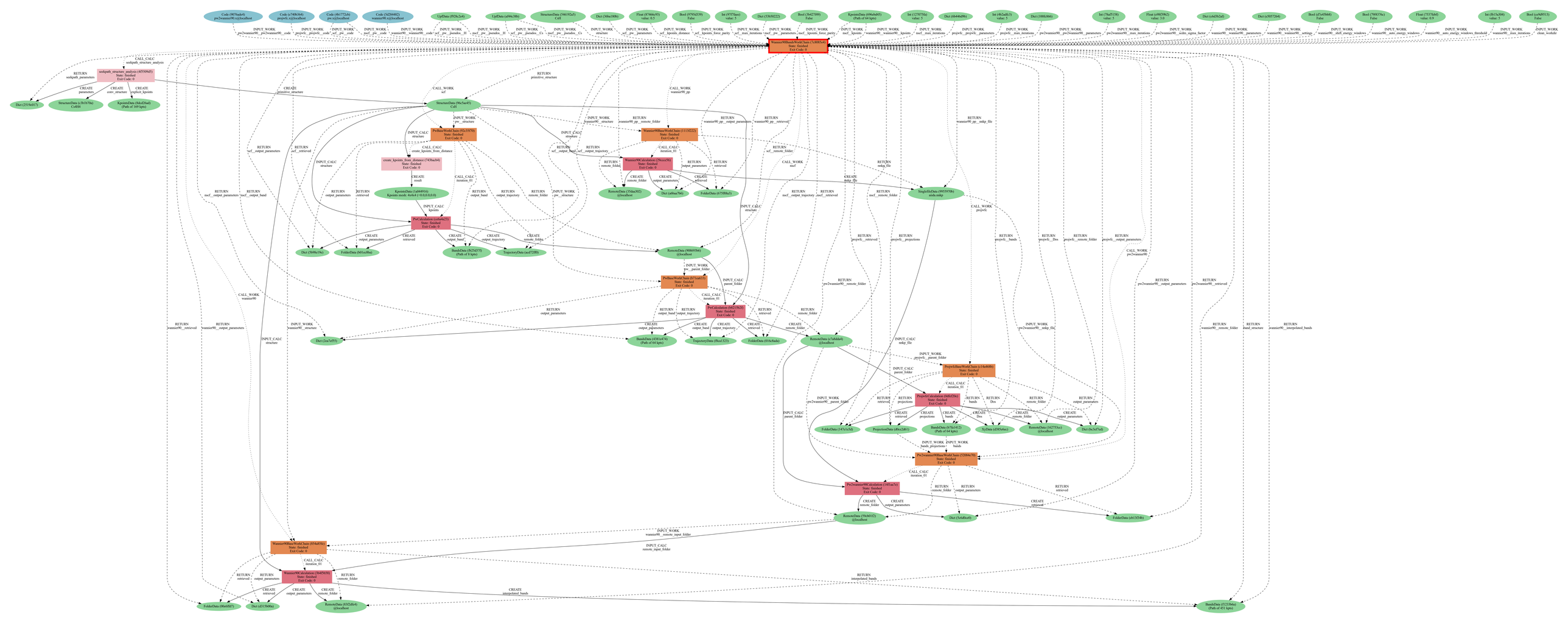

Code (9076ade4)
pw2wannier90.x@localhost
Code (e740b364)
projwfc.x@localhost
Code (4b1772cb)
pw.x@localhost
Code (5d284482)
wannier90.x@localhost
UpfData (f928c2e4)
UpfData (af44c38b)
StructureData (546192a5)
CsH
Dict (36ba180b)
Float (87466c93)
value: 0.5
Bool (9795d339)
False
Int (97f7faee)
value: 5
Dict (53b50222)
Bool (3b427f49)
False
KpointsData (696ebd45)
(Path of 64 kpts)
Int (127075fa)
value: 5
Dict (6b446d9b)
Int (4b2adfc3)
value: 5
Dict (100fc866)
Int (78af5158)
value: 5
Float (e98f39b2)
value: 3.0
Dict (c6d3b2af)
Dict (e5057264)
Bool (d7e45bb8)
False
Bool (79f4376c)
False
Float (7537febf)
value: 0.9
Int (fb15a304)
value: 5
Bool (ce9d9513)
False
INPUT_WORK
pw2wannier90__pw2wannier90__code
INPUT_WORK
projwfc__projwfc__code
INPUT_WORK
scf__pw__code
INPUT_WORK
nscf__pw__code
INPUT_WORK
wannier90__wannier90__code
INPUT_WORK
scf__pw__pseudos__H
INPUT_WORK
nscf__pw__pseudos__H
INPUT_WORK
scf__pw__pseudos__Cs
INPUT_WORK
nscf__pw__pseudos__Cs
INPUT_WORK
structure
INPUT_WORK
scf__pw__parameters
INPUT_WORK
scf__kpoints_distance
INPUT_WORK
scf__kpoints_force_parity
INPUT_WORK
scf__max_iterations
INPUT_WORK
nscf__pw__parameters
INPUT_WORK
nscf__kpoints_force_parity
INPUT_WORK
nscf__kpoints
INPUT_WORK
wannier90__wannier90__kpoints
INPUT_WORK
nscf__max_iterations
INPUT_WORK
projwfc__projwfc__parameters
INPUT_WORK
projwfc__max_iterations
INPUT_WORK
pw2wannier90__pw2wannier90__parameters
INPUT_WORK
pw2wannier90__max_iterations
INPUT_WORK
pw2wannier90__scdm_sigma_factor
INPUT_WORK
wannier90__wannier90__parameters
INPUT_WORK
wannier90__wannier90__settings
INPUT_WORK
wannier90__shift_energy_windows
INPUT_WORK
wannier90__auto_energy_windows
INPUT_WORK
wannier90__auto_energy_windows_threshold
INPUT_WORK
wannier90__max_iterations
INPUT_WORK
clean_workdir
Wannier90BandsWorkChain (7c8085e4)
State: finished
Exit Code: 0
CALL_CALC
seekpath_structure_analysis
RETURN
seekpath_parameters
seekpath_structure_analysis (4f5509d5)
State: finished
Exit Code: 0
CREATE
parameters
CREATE
conv_structure
CREATE
explicit_kpoints
CREATE
primitive_structure
Dict (2519c017)
StructureData (c3b1b70a)
Cs4H4
KpointsData (8dcd26ad)
(Path of 169 kpts)
RETURN
primitive_structure
CALL_WORK
scf
StructureData (96c5ae45)
CsH
INPUT_WORK
pw__structure
PwBaseWorkChain (92c35f70)
State: finished
Exit Code: 0
INPUT_CALC
structure
CALL_CALC
create_kpoints_from_distance
create_kpoints_from_distance (743bacb4)
State: finished
Exit Code: 0
CREATE
result
KpointsData (1a044916)
Kpoints mesh: 4x4x4 (+0.0,0.0,0.0)
INPUT_CALC
kpoints
CALL_CALC
iteration_01
RETURN
scf__output_parameters
RETURN
scf__retrieved
INPUT_CALC
structure
RETURN
output_parameters
RETURN
retrieved
RETURN
output_band
RETURN
output_trajectory
RETURN
remote_folder
RETURN
nscf__output_parameters
RETURN
nscf__output_band
PwCalculation (ce6a4a23)
State: finished
Exit Code: 0
CREATE
output_parameters
CREATE
retrieved
CREATE
output_band
CREATE
output_trajectory
CREATE
remote_folder
Dict (5b98e19e)
FolderData (b01ec8ba)
BandsData (fb25d37f)
(Path of 8 kpts)
TrajectoryData (acd72ff0)
CALL_WORK
wannier90_pp
INPUT_WORK
wannier90__structure
RETURN
wannier90_pp__remote_folder
RETURN
wannier90_pp__output_parameters
RETURN
wannier90_pp__retrieved
Wannier90BaseWorkChain (1113f222)
State: finished
Exit Code: 0
INPUT_CALC
structure
RETURN
scf__output_band
RETURN
scf__output_trajectory
CALL_CALC
iteration_01
RETURN
remote_folder
Wannier90Calculation (29ccce56)
State: finished
Exit Code: 0
RETURN
output_parameters
RETURN
retrieved
CREATE
remote_folder
CREATE
output_parameters
CREATE
retrieved
CREATE
nnkp_file
RemoteData (35daa302)
@localhost
Dict (a6baa7b6)
FolderData (675f88a3)
RETURN
scf__remote_folder
CALL_WORK
nscf
RETURN
nnkp_file
RETURN
wannier90_pp__nnkp_file
SinglefileData (9955970b)
aiida.nnkp
INPUT_WORK
pw__structure
INPUT_CALC
structure
RETURN
nscf__output_trajectory
RETURN
nscf__retrieved
RETURN
nscf__remote_folder
CALL_WORK
projwfc
RETURN
projwfc__retrieved
RETURN
projwfc__projections
RETURN
projwfc__bands
RETURN
projwfc__Dos
RETURN
projwfc__remote_folder
RETURN
projwfc__output_parameters
CALL_WORK
pw2wannier90
RemoteData (908693b6)
@localhost
INPUT_WORK
pw__parent_folder
INPUT_CALC
parent_folder
PwBaseWorkChain (b71ea633)
State: finished
Exit Code: 0
CALL_CALC
iteration_01
RETURN
output_parameters
RETURN
output_band
RETURN
output_trajectory
RETURN
retrieved
RETURN
remote_folder
PwCalculation (b8215b2f)
State: finished
Exit Code: 0
CREATE
output_parameters
CREATE
output_band
CREATE
output_trajectory
CREATE
retrieved
CREATE
remote_folder
Dict (2ea7ef55)
BandsData (4381e474)
(Path of 64 kpts)
TrajectoryData (f8ca1323)
FolderData (016c8ada)
RemoteData (e7a8dda4)
@localhost
RETURN
pw2wannier90__remote_folder
RETURN
pw2wannier90__output_parameters
RETURN
pw2wannier90__retrieved
RETURN
wannier90__remote_folder
RETURN
band_structure
RETURN
wannier90__interpolated_bands
INPUT_WORK
pw2wannier90__nnkp_file
INPUT_CALC
nnkp_file
INPUT_WORK
projwfc__parent_folder
ProjwfcBaseWorkChain (c14a468b)
State: finished
Exit Code: 0
INPUT_CALC
parent_folder
CALL_CALC
iteration_01
INPUT_WORK
pw2wannier90__parent_folder
RETURN
retrieved
RETURN
projections
ProjwfcCalculation (0dfef20e)
State: finished
Exit Code: 0
RETURN
bands
RETURN
Dos
RETURN
remote_folder
RETURN
output_parameters
INPUT_CALC
parent_folder
CREATE
retrieved
CREATE
projections
CREATE
bands
CREATE
Dos
CREATE
remote_folder
CREATE
output_parameters
FolderData (147e1e5d)
ProjectionData (d0ce2d61)
BandsData (b7fa1412)
(Path of 64 kpts)
XyData (d385e6ec)
RemoteData (162753cc)
@localhost
Dict (bc3ef7ed)
INPUT_WORK
bands_projections
INPUT_WORK
bands
Pw2wannier90BaseWorkChain (52084e70)
State: finished
Exit Code: 0
CALL_CALC
iteration_01
Pw2wannier90Calculation (14f1aa7e)
State: finished
Exit Code: 0
RETURN
remote_folder
RETURN
output_parameters
RETURN
retrieved
CREATE
remote_folder
CREATE
output_parameters
CREATE
retrieved
RemoteData (59cb01f2)
@localhost
Dict (5c6d0ce0)
FolderData (eb13f34b)
CALL_WORK
wannier90
RETURN
wannier90__retrieved
RETURN
wannier90__output_parameters
INPUT_CALC
structure
INPUT_WORK
wannier90__structure
INPUT_WORK
wannier90__remote_input_folder
INPUT_CALC
remote_input_folder
Wannier90BaseWorkChain (854a85fe)
State: finished
Exit Code: 0
CALL_CALC
iteration_01
RETURN
retrieved
RETURN
output_parameters
RETURN
remote_folder
Wannier90Calculation (3b4f5658)
State: finished
Exit Code: 0
CREATE
retrieved
CREATE
output_parameters
CREATE
remote_folder
CREATE
interpolated_bands
RETURN
interpolated_bands
FolderData (00e6ffd7)
Dict (d315b00a)
RemoteData (83f2dfe4)
@localhost
BandsData (f1233b6a)
(Path of 451 kpts)