Electronic structure E-CAM modules II

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Contents

Executive Summary

In this report for Deliverable 2.3 of E-CAM, 9 software modules in electronic structure, which are related to an Extended Software Development Workshop (ESDW) held by E-CAM and the centre for Computational Design and Discovery of Novel Materials MARVEL in San Sebastian in September 2016, are presented.

These modules are intended to be exploited during the development process of new applications that span most of the electronic structure community, but the main focus are codes that augment the capability of the Wannier90 program, both towards the interoperability (via interfaces to other programs) and towards the development of new core routines. The modules presented here are not directly related to electron-phonon calculations. Recently, some work has been done in this direction and it will be included into the next batch of modules for WP2.

These 9 modules are respectively named:

- `Symmetry-adapted Wannier functions`,
- `Wannier90-TB-interface`,
- `Adaptively-refined-mesh`,
- `Non-collinear spin`,
- `Use-WS-distance`,
- FORD `documentation tool integration`,
- `Improvements Wannier90 Z2 pack interface`,
- `Improvements Makefile`,
- `Test-suite Travis-CI integration`.

These include codes for improving the symmetry of Wannier functions (WFs), for increasing the accuracy of results while maintaining the computational cost with adaptively refined meshes, for the correct treatment of spin-orbit interaction and their documentation. In addition to these core modules, other interface layer modules are also present in this document, that extends the capability of Wannier90 to other codes.

A short description is written for each module as well as the codes where they have been implemented. The source code related to each module may be found in the Wannier90 repository under Github, with the relevant `Pull-Requests` on the GitHub repository linked within each of the documentation modules.

1 Introduction

Work Package 2 of E-CAM focuses on selecting software functionalities that are common to many electronic structure implementations, are important for the implementation and efficiency of codes, and mature enough to allow for a good definition of standards and interfaces.

Starting from an E-CAM ESDW in San Sebastian organized by the Wannier90 developers, a set of 9 modules were produced to meet the desire of the electronic-structure community to extend the use of WFs, and in particular of Maximally Localised Wannier Functions (MLWFs), to a broader class of physical and chemical problems by adding new functionality to the Wannier90 code.

The reasons for such interest are numerous: Wannier functions are an important class of functions which enable us to obtain a real-space picture of the electronic structure of a system. They provide an insightful chemical analysis of the nature of bonding, and chemical reaction in condensed-matter physics, similar to the role played by localized molecular orbitals in chemistry. They are also a powerful tool in the study of dielectric properties via the modern theory of polarisation.

More interestingly, in the condensed-matter community WFs are employed in the construction of model Hamiltonians for, e.g., correlated-electron and magnetic systems (to study new quantum phases of matter). Furthermore, WFs are used as building blocks in first-principles TB Hamiltonians, where chemically accurate Hamiltonians are constructed directly on the Wannier basis, rather than fitted or inferred from macroscopic considerations[7].

The understanding of many other phenomena of solid-state physics has been greatly influenced by the theory of WFs, such as phonons, photonic crystals and cold-atom lattices[7]. Wannier90[9] is a program that, for a given system, generates the Wannier functions with minimum spatial spreads, known as MLWFs, among the class of all possible WFs. The locality of MLWFs can be exploited to compute, among other things, band-structure, density of states and Fermi surfaces at modest computational cost. The original 2008 paper[9] describing the method has been cited 1176 times, the 2012 Review on Rev. Mod. Physics[7] 631 times and the 2014 paper[10] on the subsequent additions to the code 120 times[2]. Moreover, Wannier90 has been interfaced with many DFT codes, e.g. `QuantumEspresso`, `SIESTA` ,`VASP` etc. covering probably of the order of 10,000 users or more (see section 1.2).

Accordingly, software development in the first year of E-CAM activity has focused on extending the capability of Wannier90 both in terms of core functionalities and in terms of its ability to interface with other codes. In addition to this, work was also done on maintaining existing developments and on improving the parallel performance of the program.

The module developments are done on Wannier90's `GitHub` repository. In order to document each module, a module documentation directory is created in an E-CAM GitLab repository dedicated to Electronic Structure which automatically updates documentation for the E-CAM Electronic Structure Module Documentation on Read the Docs. A detailed contribution procedure is available through the documentation repository.

In section 2, a short description is provided for each module created, followed by a link to the `Pull-request` on GitHub of Wannier90. More detailed information about code development, testing and documentation can be found there. Additionally, we also point to the Density Functional Theory (DFT) codes already interfaced with some of these modules.

1.1 Overall scope of the module set

Engineering materials for technological applications, or of new drugs, relies on our ability to describe and manipulate matter at a microscopic level. To do this, it is essential to know how atoms interact to form molecules and more complex materials. Several approximate methods exist to tackle the problem, from very accurate and computationally demanding quantum chemistry methods to less accurate and very fast coarse-grain methods. Currently, the best compromise between efficiency and accuracy is provided by DFT, which has been successfully applied to determine a wide range of properties of atoms, molecules, and materials.

However, it is often the case, that a better understanding of electronic phenomena in materials may be achieved by looking at the electronic structure in real space. This can be obtained by performing a Wannier transformation of the Kohn-Sham (KS) orbitals (which are the default outcome of DFT calculations).

Hence, WFs play a role complementary to DFT in the understanding of many phenomena and are often employed within the electronic-structure community. Moreover, WFs provide a powerful tool to link DFT calculations to more accurate quantum calculations, such as *ab initio* Tight Binding (TB), single particle Green's function (G) and screened Coulomb potential (W) (GW) and Dynamical mean field theory (DMFT).

[2] All the citation statistics have been obtained with Google Scholar on 03/10/2017

1.2 General applications and possible exploitation of the codes

All the modules described in this deliverable are not stand-alone programs, but are instead intended to be used from within the Wannier90 code which has in turn interfaces with many DFT and TB codes. They are distributed under the same GNU General Public licence used for the Wannier90 program.

Wannier90 is used as a postprocessing tool. Therefore, the end users of electronic-structure codes, such as DFT, TB, QMC codes, that are interfaced with these modules via Wannier90, will benefit from the functionalities they provide, e.g. Wannier functions with improved symmetry, spin-orbit calculations etc., and they can focus on developing new ideas, and new science without needing to rewrite functionalities that are already established.

Several popular electronic structure codes are already interfaced with Wannier90. The ones we are aware of, in no particular order, are:

- `QUANTUMESPRESSO`[3] is a suite of Open-Source for electronic-structure calculations. It is based on DFT, plane waves, and pseudopotentials. It is now integrated and distributed with the Schrödinger's Materials Science Suite. `QUANTUMESPRESSO` is one of the most used Open-Source DFT codes worldwide.
- `SIESTA`[11] is a computer program to perform efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids, based on linear-scaling algorithms. The SIESTA program is distributed freely to academics and has a large basin of user in different research fields, such as geosciences, biology, and engineering (apart from those in its natural habitat of materials physics and chemistry). Currently there are several thousand users all over the world, and the paper describing the method[11] has received more than 6000 citations so far.
- WIEN2k is a program package[1] that allows to perform electronic structure calculations of materials using DFT. It is based on the full-potential augmented plane-wave (L APW) plus local orbitals method. More than 2000 user groups have been licensed so far.
- GPAW[8] is an Open-Source DFT Python code based on the projector-augmented wave (PAW) method and the atomic simulation environment (ASE). It is now supported by the European project NOMAD.
- `abinit`[5] is a software suite to calculate several properties of materials. The core quantum equations are those of DFT, perturbation theories based on DFT, and many-body Green's functions (GW and DMFT).
- `OpenMX` is a software package for material simulations based on linear-scaling density functional theory, and localised basis functions. Systems consisting of tens of thousands of atoms are possible with the method implemented in OpenMX if several thousands cores on a parallel computer are available. The distribution of the program package and the source codes follow the practice of the GNU General Public License (GPL).
- `VASP`[6] is a computer program for atomic scale materials modelling, e.g. electronic structure calculations and quantum-mechanical molecular dynamics, based on DFT. It is one of the most employed commercial DFT codes worldwide.
- `PythTB` is a Python software package implementing the TB approximation. It is used to build and solve tight-binding models of the electronic structure of systems of arbitrary dimensionality (crystals, slabs, ribbons, clusters, etc.).

2 Modules

In this section, a short description is written for each module, followed by a link to the `Pull-Request` on `GitHub`, which shows detailed information about code development, testing and documentation.

2.1 Symmetry Adapted Wannier functions

`Symmetry Adapted Wannier Functions` is a module within Wannier90 which is devoted to the construction of Wannier function with a given symmetry. The procedure implemented in this module enables one to control the symmetry and center of the Wannier functions and also simplifies the minimization of the spread functional under these symmetry constraints.

2.1.1 Practical application and exploitation of the code

This module is accessible through the Wannier90 code, which in turn is interfaced with the all the most popular DFT codes. This module has been used to study the properties of strongly correlated materials and to assess the quality of high-level quantum methods[2].

Direct Documentation Link	readme.rst of Symmetry Adapted Wannier Functions module.

2.2 Non-collinear Spin

`Non-collinear Spin` is a module that enables one to perform non-collinear spin calculations with ultrasoft pseudopotentials functionality.

2.2.1 Practical application and exploitation of the code

This module is accessible through Wannier90, which in turn is interfaced with the all the most popular DFT codes. Non-collinear spin calculations are crucial to study the magnetic properties of many metals and oxides. With this module is now possible to couple Wannier90 to DFT calculations that make use of ultrasoft pseudopotentials to reduce the computational overload.

Direct Documentation Link	readme.rst of Non-collinear spin module.

2.3 Use_WS_distance

`Use_WS_distance` is a module implemented to exploit the Wigner-Seitz distance[4] during the interpolation of band structures. In particular, it helps to improve the interpolation of bandstructures in the more general case when the centres of the Wannier functions are not necessarily close to the R=0 unit cell.

2.3.1 Practical application and exploitation of the code

This module is part of the Wannier90 code. It is used in bandstructure interpolation for accurate determination of electronic structure properties of materials.

Direct Documentation Link	readme.rst of Use_WS_distance module.

2.4 Wannier90-TB interface modules

This module allows tight-binding parameters, including Hamiltonian matrix elements and matrix elements of the position operator in the Wannier function basis, to be generated and output from Wannier90.

2.4.1 Practical application and exploitation of the code

It is particularly useful for larger scale and/or correlated tight-binding models of materials, for use with TB codes such as pythtb, that enable calculations beyond the current capabilities of conventional density-functional theory calculations.

Direct Documentation Link	readme.rst of Wannier90-TB interface module.

2.4.2 Adaptively-refined-mesh

This module enables properties defined in the Brillouin zone, such an interpolated band structures, to be calculated on grids/meshes that have a density that is refined adaptively rather than fixed.

2.4.3 Practical application and exploitation of the code

More accurate interpolation of Brillouin zone properties such as interpolated bandstructures.

Direct Documentation Link	readme.rst of Adaptively-refined-mesh module.

2.4.4 FORD-documentation-tool-integration

This is a module that systematises the internal documentation of the Wannier90 code using the FORD documentation system.

2.4.5 Practical application and exploitation of the code

Improved sustainability of software development for the developer community.

Direct Documentation Link	readme.rst of FORD-documentation-tool-integration module.

2.5 Improvement-Wannier90-Z2Pack-interface

This module enables Wannier90 to output matrix elements relevant for computing topological invariants of materials such as topological insulators.

2.5.1 Practical application and exploitation of the code

The code is interfaced with the Z2Pack (link).

Direct Documentation Link	readme.rst of Improvement-Wannier90-Z2Pack-interface module.

2.6 Improvements-Makefile

This module involves significant improvements to the make system for the code to enable smooth and robust compilation on a variety of computer platforms.

Direct Documentation Link	readme.rst of Improvements-Makefile module.

2.7 Test-suite-Travis-CI-Integration

This module implements automatic regression testing of the code and automatic testing of pull requests.

2.7.1 Practical application and exploitation of the code

Improved robustness of software development and software sustainability.

Direct Documentation Link	readme.rst of Test-suite-Travis-CI-Integration module.

3 Outlook

The report of Deliverable 2.3 of E-CAM describes 9 Software modules in electronic structure related to the ESDW San Sebastian. They include developments for the Wannier90 program and its interface with other electronic structure codes. In particular, as outlined in Sec. 2, these modules deal with the implementation of symmetry adapted Wannier functions, to improve the symmetery of the Wannier functions and related electronic-structure quantities, such as band structure and density of states; improvements in the interpolation of band structures, developments in the selection of the k-point mesh to increase accuracy, ability of performing non-collinear spin calculations as well as interface layer modules to tight-binding codes. We believe that the electronic structure community will greatly benefit from these and future developments, as confirmed by the increasing number of citations of the Wannier90 code.

Modules explicitly designed to improve the performance of electron phonon calculations with Wannier functions are part of future developments. Some preliminary work has already been done in this direction and it will be presented in the next batch of modules.

References

Acronyms Used

CECAM Centre Européen de Calcul Atomique et Moléculaire

TB Tight Binding

DFT Density Functional Theory

WS Wigner-Seitz

WFs Wannier functions

ESDW Extended Software Development Workshop

MLWFs Maximally Localised Wannier Functions

FORD FORtran Documented

DMFT Dynamical mean field theory

KS Kohn-Sham

GW single particle Green's function (G) and screened Coulomb potential (W)

QMC Quantum Monte Carlo

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