An updated version of wannier90: A tool for obtaining maximally-localised Wannier functions

Arash A. Mostofi; Jonathan R. Yates; Giovanni Pizzi; Young-Su Lee; Ivo Souza; David Vanderbilt; Nicola Marzari

New version program summary

Program title: wannier90

Catalogue identifier: AEAK_v2_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEAK_v2_0.html

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

Licensing provisions: GNU General Public License, version 2

No. of lines in distributed program, including test data, etc.: 930 386

No. of bytes in distributed program, including test data, etc.: 47 939 902

Distribution format: tar.gz

Programming language: Fortran90, perl.

Computer: Any architecture with a Fortran 90 compiler.

Operating system: Linux, Windows, Solaris, AIX, Tru64 Unix, OSX.

Has the code been vectorised or parallelized?: Yes, parallelized using MPI.

RAM: 10 Mb

Classification: 7.3.

External routines:

- BLAS (http://www/netlib.org/blas)
- LAPACK (http://www.netlib.org/lapack)
- MPI libraries (optional) for parallel execution

Catalogue identifier of previous version: AEAK_v1_0

Journal reference of previous version: Comput. Phys. Comm. 178(2008)685

Does the new version supersede the previous version?: Yes

Nature of problem:

Obtaining maximally-localised Wannier functions from a set of Bloch energy bands that may or may not be entangled, and using these Wannier functions to calculate electronic properties of materials. Solution method: In the case of entangled bands, the optimally-connected subspace of interest is determined by minimising a functional which measures the subspace dispersion across the Brillouin zone. The maximally-localised Wannier functions within this subspace are obtained by subsequent minimisation of a functional that represents the total spread of the Wannier functions in real space. For the case of isolated energy bands only the second step of the procedure is required.

Reasons for new version:

Addition of new functionality, minor bug fixes, and parallel (MPI) execution for parts of the code. Summary of revisions:

Enhancements include:

• Spinor projections

• Improved plotting

• Parallel execution

• Calculation of van der Waals interactions

• Landauer–Buttiker and Boltzmann transport

Full details are given in the CHANGE.log file, which can be found in the root directory of the distribution.

Additional comments:

The distribution file for this program is over 47 MB and therefore is not delivered directly when Download or Email is requested. Instead a html file giving details of how the program can be obtained is sent.

Running time:

Example calculations run in a few minutes.