General information about the FPLO code

FPLO is an all-electron, **F**ull-**P**otential, **L**ocal-**O**rbital electronic structure code [1] using a fixed atomic-like basis set [2]. It allows to treat bulk systems with 3-dimensional periodic boundary conditions and molecules/clusters with free boundary conditions on equal footing, i.e., with the same kind of basis.

Three different iteration schemes allow to converge the Kohn-Sham equations even in critical cases. As a whole, the code is designed for easy handling, high accuracy, efficiency, and stability of the numerics. It allows for calculations with structural units including up to 300 atoms on single-CPU machines.

Relativistic effects are implemented in four different variants (non-relativistic, scalar relativistic [two variants], full relativistic [four component Dirac]) [3]. Optimization of atomic positions via calculation of forces is implemented for the non-relativistic and for the scalar relativistic modes. The quantization axis is variable in the case of full relativistic spin polarized calculations.

LSDA+*U* and GGA+*U* are implemented for two different functionals (around mean field and atomic limit, for details see the overview in Ref. [4]) and for two different projections, in all four relativistic modes. The orbital polarization correction is implemented in two variants (spin dependent [5] and spin independent [6]).

Fixed spin moment calculations [7] are implemented for all four relativistic modes.

Further features:

- Finite nuclei;
- Charged systems: virtual crystal approximation, jellium, and molecular charge;
- Open core calculations for 4f systems or simulation of core holes;
- Calculation of optical spectra (not in full relativistic mode);
- De Haas – van Alphen module;
- Scaling of the exchange field ("LSDA•x");
- Band structure plots on symmetry lines, including so-called fat bands (band weights);
- Band-unfolding for the interpretation of ARPES data;
- Projected densities of states with variable quantization axis;
- Molecular-orbital projected density of states and band weights;
- Wannier function module (maximally projected Wannier functions):
    * local spin axes can be defined for each projector;
    * spin-mixed relativistic Wannier functions;
- Topological insulators: Z_2 invariants for all systems;
- Weyl semi metals: determination of Weyl points;
- Calculation of surface states from Wannier models;
- Module pyfplo for scripting and input manipulation;

- Module xfplo:

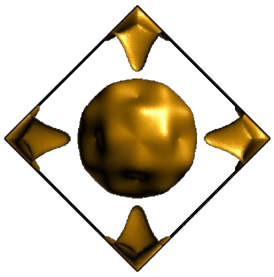
    * visualization of structures and Fermi surfaces;

    * structure and symmetry manipulation;

    * cif importer;

    * display of Wannier functions and grid output functions (density, spin-density, potential, Bloch wave functions and energy-resolved densities on flexible grids);

    * visual Brillouin zone – path construction with automatic point labels for all symmetries in the Fermi surface mode.



Enjoy FPLO!

Dresden, January 2018. The developers.

References:

[1] K. Koepernik and H. Eschrig, Phys. Rev. B 59, 1743 (1999).

[2] M. Richter, K. Koepernik, and H. Eschrig, in: Condensed Matter Physics in the Prime of the 21st Century (43rd Karpacz Winter School of Theoretical Physics Ladek Zdroj, Poland, 5-11 February 2007), Ed. J. Jedrzejewski, World Scientific, Singapore 2008, pp. 271-291, ISBN-13 978-981-270-944-8.

[3] H. Eschrig, M. Richter, and I. Opahle, in: Relativistic Electronic Structure Theory - Part II: Applications, ed. by P. Schwerdtfeger, Elsevier, Amsterdam 2004, pp. 723-776.

[4] E. R. Ylvisaker, W. E. Pickett, and K. Koepernik, Phys. Rev. B **79**, 035103 (2009).

[5] L. Nordström, M. S. S. Brooks, and B. Johansson, J. Phys C **4**, 3261 (1992).

[6] O. Eriksson, M. S. S. Brooks, and B. Johansson, Phys. Rev. B **41**, R7311 (1990).

[7] K. Schwarz and P. Mohn, J. Phys. F: Met. Phys. **14**, L129 (1984).