General information about the FPLO code

FPLO is an all-electron, Full-Potential, Local-Orbital 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: