General information about the FPLO code

FPLO is an all-electron, **F**ull-**P**otential, **L**ocal-**O**rbital electronic structure code [1] using an atomic-like basis set with fixed radial wave functions [2]. The FPLO package allows to carry out DFT-based calculations on 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 set. In addition, the package comprises a free atom / ion DFT code with relaxed radial wave functions.

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 [3], efficiency, and stability of the numerics [4]. 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]) [5]. 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 (collinear spin approximation).

Beyond the standard L(S)DA and GGA functionals, the modified Becke-Johnson functional is implemented. Also, LSDA+*U* and GGA+*U* are implemented for two different double countings (around mean field and atomic limit, for details see the overview in Ref. [6]) and for two different projections, in all four modes of relativistic treatment. The orbital polarization correction is implemented in two variants (spin dependent [7] and spin independent [8]).

Fixed spin moment calculations [9] are implemented for all four modes of relativistic treatment.

Further features:

- Finite nuclei;
- Charged or doped systems: virtual crystal approximation, jellium, and molecular charge;
- Open core calculations for 4f systems or simulation of core holes;
- Simple extension or modification of the basis set;
- Reciprocal space integrations with linear tetrahedron method (with Blöchl corrections) or broadening schemes, using optimized k-meshes;
- 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, input manipulation, data extraction, and topology calculation;
- Module xfplo:
    * visualization of structures and Fermi surfaces;
    * structure and symmetry manipulation;
    * cif importer and exporter;
    * 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, July 2022. The developers.

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