This is the 2018 release of FPLO which comes with a number of new features:

- input:

* =.sym has been removed, only =.in is needed.
* fedit is now tightly bound to the fplo version. This means that it is hard linked against the input management libraries of the corresponding version. The option -p has been removed.

- topological insulators: Z_2 invariants are implemented for all systems

- Weyl semi metals: determination of Weyl points, calculation of surface states from Wannier models, ... (pyfplo module slabify)

- pyfplo (scripting, input manipulation, use Wannier functions to calculate surface states, idealized slabs,... ; read FPLO.../DOC/pyfplo/pyfplo.pdf)

- pyxfbp (python bindings for xfbp)

- dHvA module

- Wannier function module:

* local spin axes can be defined for each projector
* spin-mixed relativistic Wannier functions should work now
* real space representation of WFs can be loaded into xfplo
* new output file +hamdata for use in pyfplo.slabify

- xfplo:

* new enhanced symmetry settings
* symmetry manipulation
* cif importer
* atom labels
* display Wannier functions and grid output functions
* visual BZ-path construction with automatic point labels for all symmetries in the Fermi surface mode (import/export to =.in)

Please read the section "Summary of changes" in FPLO.../DOC/MANUAL/doc.pdf (part of the distribution) for links to further information.

Warning: The new symmetry treatment is more general. Old projects and new projects may not be compatible. Especially site coordinates might be different (although equivalent), which matters for difvecs in =.wandef and =.bwdef. This should not affect completely new projects.

Topological invariants for inversion symmetric systems might look different: we print the invariants after each Kramers pair. The new symmetry module can contain trivial shifts in the non-symmorphic translations (compared to the old symmetry module). Such shifts can lead to sign changes of the δ_i at the TRIM points. If the changes take place inside a fourfold degenerate manifold with mixed parities (for some non-symmorphic space group irreps on the zone boundary) this sign change is not applied in the old order. Hence, the printed invariants change. However, in this case they do not have a meaning (no gap). So, no harm done.

Dresden, January 2018.

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