

# BEEF Functional Software

## libbeef Library

Johannes Voss has ported BEEF [1] (Bayesian Error Estimation Functional) to both Quantum Espresso and VASP. In both cases a small library called `libbeef` must be built.

Version	Source Code	Precompiled Linux 64-bit binary
0.1.1	<a href="#">libbeef-0.1.1.tar.gz</a>	<a href="#">libbeef-0.1.1-gcc-x86_64.tar.gz</a>

The latest development version can be obtained with this command:

```
git clone https://github.com/vossjo/libbeef
```

Installation instructions for the different versions are contained in the README file in the above downloadable files.

## Espresso with BEEF

Installation instructions (including an ASE python interface) can be found here:

<https://github.com/vossjo/ase-espresso/wiki>

## VASP with BEEF

Newer versions of VASP (V. 5.4.x and up) only need changes to the makefile to enable the BEEF functionals: add `-Dlibbeef` to the CPP flags and `-Lproperpath -lbeef` to the library linker flags.

For older versions of VASP, a patch file must now be applied to the appropriate unmodified version of the VASP source code. The patch files can be downloaded from here:

VASP Version	Patch File
5.3	<a href="#">vasp.5.3.beef.diff</a>

Apply the patch within the VASP directory containing the fortran files by executing a command like:

```
patch -p1 < vasp.5.3.beef.diff
```

Then add the following to your Makefile line where the `LIB` variable is defined:

```
-Lpathtobeeflibrary/lib -lbeef
```

Then build VASP as usual. The following lines should be appended to your `.INCAR` file to run a BEEF calculation (the last line is optional and triggers the calculation of ensemble energies for error estimation):

```
GGA = BF
LUSE_VDW = .TRUE.
Zab_VDW = -1.8867
LBEEFENS = .TRUE.
```

Instructions for doing the error estimations in VASP can be found in the `libbeef` README file.

[1] Jess Wellendorff, Keld T. Lundgaard, Andreas Møgelhøj, Vivien Petzold, David D. Landis, Jens K. Nørskov, Thomas Bligaard, and Karsten W. Jacobsen, "Density functionals for surface science: Exchange-correlation model development with Bayesian error estimation", Phys. Rev. B 85, 235149 (2012).