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 `lib beef` must be built.

Version	Source Code	Precompiled Linux 64-bit binary
0.1.1	libbeef-0.1.1.tar.gz	libbeef-0.1.1-gcc-x86_64.tar.gz

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	vasp.5.3.beef.diff

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).