

VASP 6.1.0 版本编译报错及解决

1. 报错内容:

```
fftmpiw.F(38): error #5102: Cannot open include file 'fftw3.f'
      include 'fftw3.f'
      ^
fftmpiw.F(94): error #5102: Cannot open include file 'fftw3.f'
      include 'fftw3.f'
      ^
fftmpiw.F(122): error #5102: Cannot open include file 'fftw3.f'
      include 'fftw3.f'
      ^
fftmpiw.F(392): error #5102: Cannot open include file 'fftw3.f'
      include 'fftw3.f'
      ^
compilation aborted for fftmpiw.f90 (code 1)
make[2]: *** [fftmpiw.o] Error 1
make[2]: Leaving directory `/public/home/weiqi/apps/vasp.6.1.0/build/std'
cp: cannot stat 'vasp': No such file or directory
make[1]: *** [all] Error 1
```

解决:

修改 makefile.include 文件:

```
#INCS      =-I$(MKLRROOT)/include/fftw      → 修改前
FFTW       = /public/software/mathlib/fftw/3.3.4/float
LLIBS      += -L$(FFTW)/lib -lfftw3      → 修改后
INCS       += -I$(FFTW)/include
```

fftw 库的默认路径是 intel 编译器自带的, 修改为集群上单独安装的 fftw 库之后编译成功