vasp安装

计算软件安装笔记

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1.基本
cd
tar -vzxf vasp.5.4.4.tar.gz（解压vasp）
cd vasp.5.4.4
cp arch/makefile.include.linux\_intel .（把子文件夹makefile.include.linux\_intel复制到本文件夹，注意句末的点）
mv makefile.include.linux\_intel makefile.include（重命名）
vi makefile.include
i（打开编译模式）
在 OFLAG=-O2 行后加上 -xhost

OFLAG=-O2 行后加上 -xhost是针对AVX指令集的CPU。对于AMD的CPU，建议不加；对于至强E5 V4以上的版本，建议加；对于intel gold及以上，建议加AVX512



Esc
:（英文状态下）
wq!
待测试
在修改第30行，并在后面加上
OBJECTS = fftmpiw.o fftmpi\_map.o fft3dlib.o fftw3d.o \
$(MKLROOT)/interfaces/fftw3xf/libfftw3xf\_intel.a
2.固定晶格基矢
在对称性允许的条件下，VASP的晶胞优化（ISIF = 3）是允许在9个自由度上自由弛豫的，如果想要固定其中几个自由度需要用重新编译过的vasp。
重写constr\_cell\_relax.F，直接覆盖./src/的文件即可
constr\_cell\_relax.F
!-----------------------------------------------------------------------
!
! At present, VASP does not allow to relax the cellshape selectively
! i.e. for instance only cell relaxation in x direction.
! To be more precisse, this behaviour can not be achived via the INCAR
! or POSCAR file.
! However, it is possible to set selected components of the stress tensor
! to zero.
! The most conveninent position to do this is the routines
! CONSTR\_CELL\_RELAX (constraint cell relaxation).
! FCELL contains the forces on the basis vectors.
! These forces are used to modify the basis vectors according
! to the following equations:
!
! A\_OLD(1:3,1:3)=A(1:3,1:3) ! F90 style
! DO J=1,3
! DO I=1,3
! DO K=1,3
! A(I,J)=A(I,J) + FCELL(I,K)\*A\_OLD(K,J)\*STEP\_SIZE
! ENDDO
! ENDDO
! ENDDO
! where A holds the basis vectors (in cartesian coordinates).
!
!-----------------------------------------------------------------------
SUBROUTINE CONSTR\_CELL\_RELAX(FCELL)
USE prec
REAL(q) FCELL(3,3)
! just one simple example
! relaxation in x directions only
! SAVE=FCELL(1,1)
! FCELL=0 ! F90 style: set the whole array to zero
! FCELL(1,1)=SAVE
! relaxation in z direction only
! SAVE=FCELL(3,3)
! FCELL=0 ! F90 style: set the whole array to zero
! FCELL(3,3)=SAVE
LOGICAL FILFLG
INTEGER ICELL(3,3)
INQUIRE(FILE='OPTCELL',EXIST=FILFLG)
IF (FILFLG) THEN
OPEN(67,FILE='OPTCELL',FORM='FORMATTED',STATUS='OLD')
DO J=1,3
READ(67,"(3I1)") (ICELL(I,J),I=1,3)
ENDDO
CLOSE(67)
DO J=1,3
DO I=1,3
IF (ICELL(I,J)==0) FCELL(I,J)=0.0
ENDDO
ENDDO
ENDIF
RETURN
END SUBROUTINE
3.编译带wannier的vasp
<https://github.com/Chengcheng-Xiao/VASP2WAN90_v2_fix>
<https://rehnd.github.io/tutorials/vasp/vasp-wannier90>
先编译wannier，使用make lib生成libwannier.a库文件
再在vasp主文件夹makefile.include文件中添加以下两行
CPP\_OPTIONS+=-DVASP2WANNIER90v2
LLIBS+=/public/software/wannier/libwannier.a

make all
多核编译可能会出问题，所以不使用make all -j 8
（完成）
使用mpirun -np 2 /root/vasp.5.4.4/bin/vasp\_std运行vasp
参考文献 https://www.bilibili.com/video/BV1MJ411q7mB

vasp+vtst
[{+}](https://theory.cm.utexas.edu/vtsttools/installation.html)https://theory.cm.utexas.edu/vtsttools/installation.html+
1 解压vasp
tar -zxvf vasp.5.4.4.tar.gz
或初始化vasp
make veryclean
2 解压vtst软件
tar -zxvf vtstcode-184.tgz
3 修改vasp编译文件
修改 (home-vasp)/src/main.F 文件
将
CALL CHAIN\_FORCE(T\_INFO%NIONS,DYN%POSION,TOTEN,TIFOR, &
LATT\_CUR%A,LATT\_CUR%B,IO%IU6)
修改为
CALL CHAIN\_FORCE(T\_INFO%NIONS,DYN%POSION,TOTEN,TIFOR, &
TSIF,LATT\_CUR%A,LATT\_CUR%B,IO%IU6)
备份(home-vasp)/src/ chain.F文件
cp chain.F chain.F\_back
修改(home-vasp)/src/. objects文件
在chain.o \ 关键词前添加
bfgs.o dynmat.o instanton.o lbfgs.o sd.o cg.o dimer.o bbm.o \
fire.o lanczos.o neb.o qm.o opt.o \
将(home-vtst)/vtstcode5/下的文件复制到(home-vasp)/src/文件夹下
cp (home-vtst)/vtstcode5/\* (home-vasp)/src/
4 编译vasp
cp arch/makefile.include.linux\_intel makefile.include
修改makefile.include文件
在 OFLAG=-O2 行后加上 -xhost



make all
vasp544+beef
beef安装包名：libbeef-0.1.1.tar.gz vasp.5.4.4.tar.gz
homedir=/public/software/vasp

1. 安装beef

module load intel/2018
tar -zxvf vasp.5.4.4.tar.gz
tar -zxvf libbeef-0.1.1.tar.gz
cd libbeef-0.1.1
./configure --prefix=/public/software/vasp/beef
make
make install
（检查在/public/software/vasp/beef/lib文件夹内有无libbeef.a）

1. 配置vasp

cd $homedir/vasp.5.4.4
cp ./arch/makefile.include.linux\_intel makefile.include
（修改makefile.include）



-Dlibbeef



-L/public/software/vasp/beef/lib -lbeef

1. 编译

make all

1. 简单使用

（INCAR添加参数）
GGA = BF
LUSE\_VDW = .TRUE.
Zab\_VDW = -1.8867
LBEEFENS = .TRUE.
参考资料
<http://wiki.tangzeyuan.com/software/vasp-compilation.html>
[https://confluence.slac.stanford.edu/display/SUNCAT/BEEF+Functional+Software](https://confluence.slac.stanford.edu/display/SUNCAT/BEEF%2BFunctional%2BSoftware)
vasp544+sol
安装包名：VASPsol-master.zip vasp.5.4.4.tar.gz
homedir=homedir=/public/software/vasp

1. sol准备

unzip VASPsol-master.zip

1. 配置vasp

tar -zxvf vasp.5.4.4.tar.gz
cd $homedir/vasp.5.4.4
cp $homedir/VASPsol-master/src/solvation.F ./src



-Dsol\_compat
cp ./src/pot.F ./src/pot.F\_back
patch ./src/pot.F < $homedir/VASPsol-master/src/patches/pbz\_patch\_541

1. 编译

make all
参考资料
<https://mp.weixin.qq.com/s/pWLNZknUvLcYKw5IAlSaZg>
<https://github.com/henniggroup/VASPsol>