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[](https://www.bilibili.com/video/BV1MJ411q7mB)  
  
vasp+vtst  
[{+}](https://theory.cm.utexas.edu/vtsttools/installation.html)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



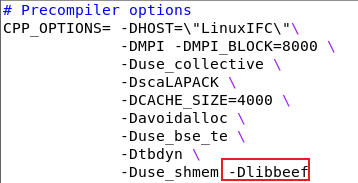
make all  
vasp544+beef  
beef安装包名：libbeef-0.1.1.tar.gz vasp.5.4.4.tar.gz  
homedir=/public/software/vasp

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

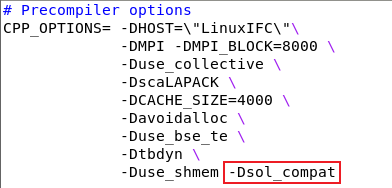
（INCAR添加参数）  
GGA = BF  
LUSE\_VDW = .TRUE.  
Zab\_VDW = -1.8867  
LBEEFENS = .TRUE.  
参考资料  
<http://wiki.tangzeyuan.com/software/vasp-compilation.html>  
<https://confluence.slac.stanford.edu/display/SUNCAT/BEEF+Functional+Software>  
vasp544+sol  
安装包名：VASPsol-master.zip vasp.5.4.4.tar.gz  
homedir=homedir=/public/software/vasp

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>