```bash
# ~/.bashrc: executed by bash(1) for non-login shells.
# see /usr/share/doc/bash/examples/startup-files (in the package
bash-doc)
# for examples

# If not running interactively, don't do anything
[ -z "$PS1" ] && return

# don't put duplicate lines in the history. See bash(1) for more
options
export HISTCONTROL=ignoreboth

# check the window size after each command and, if necessary,
# update the values of LINES and COLUMNS.
shopt -s checkwinsize

# make less more friendly for non-text input files, see lesspipe(1)
[ -x /usr/bin/lesspipe ] && eval "$(lesspipe)"

# set variable identifying the chroot you work in (used in the
prompt below)
if [ -z "$debian_chroot" ] && [ -r /etc/debian_chroot ]; then
    debian_chroot=$(cat /etc/debian_chroot)
fi

# set a fancy prompt (non-color, unless we know we "want" color)
case "$TERM" in
xterm-color)

PS1='${debian_chroot:+($debian_chroot)}\[\033[01;32m\]\u@\h\[\033[00
m\]:\[\033[01;34m\]\w\[\033[00m\]\$ '
    ;;
*)
    PS1='${debian_chroot:+($debian_chroot)}\u@\h:\w\$ '
    ;;
esac

# Comment in the above and uncomment this below for a color prompt
#PS1='${debian_chroot:+($debian_chroot)}\[\033[01;32m\]\u@\h\[\033[0
0m\]:\[\033[01;34m\]\w\[\033[00m\]\$ '

# If this is an xterm set the title to user@host:dir
case "$TERM" in
xterm*|rxvt*)
    PROMPT_COMMAND='echo -ne "\033]0;${USER}@${HOSTNAME}:
${PWD/$HOME/~}\007"'
    ;;
*)
    ;;
esac

# Alias definitions.
```

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# You may want to put all your additions into a separate file like
# ~/.bash_aliases, instead of adding them here directly.
# See /usr/share/doc/bash-doc/examples in the bash-doc package.

#if [ -f ~/.bash_aliases ]; then
#    . ~/.bash_aliases
#fi

# enable color support of ls and also add handy aliases
if [ "$TERM" != "dumb" ]; then
    eval "`dircolors -b`"
    alias ls='ls --color=auto'
    #alias dir='ls --color=auto --format=vertical'
    #alias vdir='ls --color=auto --format=long'
fi

# some more ls aliases
#alias ll='ls -l'
#alias la='ls -A'
#alias l='ls -CF'

# enable programmable completion features (you don't need to enable
# this, if it's already enabled in /etc/bash.bashrc and /etc/profile
# sources /etc/bash.bashrc).
if [ -f /etc/bash_completion ]; then
    . /etc/bash_completion
fi
module use --append $HOME/my_modules
#module load icc
#module load ifort
#module load mkl
#module load fftw/3.3.8_gcc620
#module load openmpi/4.1.0_gcc620
#module load mpich/
module load  python
#source
/home/users/mollabashi/intel/composer_xe_2013.5.192/bin/compilervars
.sh intel64
export
LD_LIBRARY_PATH=/home/users/mollabashi/expands/openmpi/lib:/home/use
rs/mollabashi/expands/fftw/lib:$LD_LIBRARY_PATH
export
PATH=/home/users/mollabashi/expands/openmpi/bin:/home/users/mollabas
hi/expands/fftw/bin:$PATH
#export
LD_LIBRARY_PATH=/opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/lib
:/opt/exp_soft/local/generic/fftw/3.3.8_gcc620/lib:$LD_LIBRARY_PATH
#export
PATH=/opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/bin:/opt/exp_s
oft/local/generic/fftw/3.3.8_gcc620/bin:$PATH
# added by WIEN2k: BEGIN
# -------------------------------------------------------
```

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alias lsi="ls -aslp *.in*"
alias lso="ls -aslp *.output*"
alias lsd="ls -aslp *.def"
alias lsc="ls -aslp *.clm*"
alias lss="ls -aslp *.scf* */*.scf"
alias lse="ls -aslp *.error"
alias LS="ls -aslp | grep /"
alias pslapw="ps -ef |grep "lapw""
alias cdw="cd /home/users/mollabashi/WIEN2k"
if [ "$OMP_NUM_THREADS" = "" ]; then export OMP_NUM_THREADS=4; fi
#export LD_LIBRARY_PATH=.....
export EDITOR="vim"
export SCRATCH=./
if [ "$WIENROOT" = "" ]; then export
WIENROOT=/home/users/mollabashi/expands/v21.1; fi
export W2WEB_CASE_BASEDIR=/home/users/mollabashi/WIEN2k
export STRUCTEDIT_PATH=$WIENROOT/SRC_structeditor/bin
export PDFREADER=xpdf
export PATH=$WIENROOT:$STRUCTEDIT_PATH:$WIENROOT/SRC_IRelast/script-
elastic:$PATH:.
export OCTAVE_EXEC_PATH=${PATH}::
export OCTAVE_PATH=${STRUCTEDIT_PATH}::

export PATH=$PATH:$WIENROOT:.
ulimit -s unlimited
alias octave="octave -p $OCTAVE_PATH"
# ----------------------------------------------------
# added by WIEN2k: END
```