Simulating STM images

Wang Materials Group

UT Austin, McKetta Department of Chemical Engineering

The objective here is to explore the possibility of simulating STM images from DFT calculations. Some references for learning the learning are given along with some practical examples with AlAs (110) and BiVO4 (010) surfaces with the postprocessing module in Quantum ESPRESSO.

1 Some Theory

1.1 Other papers and references

- G. Binnig, H. Rohrer, Ch. Gerber, and E. Weibel Phys. Rev. Lett. 49, 57 (1982) 10.1103/PhysRevLett.49.57
- Gerd Binnig and Heinrich Rohrer Rev. Mod. Phys. 59, 615 (1987) 10.1103/RevModPhys.59.615
- Tutorial and derivation of Bardeen's approach with modern interpretations: Gottlieb, A. D. & Wesoloski, L. Nanotechnology 17, R57–R65 (2006).
- C.J Chen "Introduction to Scanning Tunneling Microscopy", Ch 2
  - 10.1093/acprof:oso/9780199211500.001.0001

1.2 Ways to write the tunneling current

- Some useful group websites with summaries (for STM measurements at low temperatures and low biases)
  - Hoffman Group, Havard
  - Zelijkovic Group, Boston College
- Tersoff1985 10.1103/PhysRevB.31.805; based on Bardeen's approach

$$I = \frac{2\pi e}{\hbar} \sum_{\mu,\nu} f(E_\mu)([1 - f(E_\nu + eV)]|M_{\mu\nu}|^2 \delta(E_\mu - E_\nu)$$

- approximating the tunneling of electrons across vacuum a the transmission of electrons across a square barrier, we can write an expression for the tunneling current using WKB approximation; based on here
  - we know the solution of the wavefunction in the barrier is $\psi(x) = \psi(0)e^{-\kappa x}, \kappa = \frac{\sqrt{2m(\phi - E)}}{\hbar}$
  - the probability of finding electron past barrier of width d is $|\psi(d)|^2 = |\psi(0)|^2 e^{-2\kappa d}$
  - the definite of the local DOS is $\rho(z, E) = \frac{1}{\varepsilon} \sum_{E_n = E - \varepsilon} |\psi_n(z)|^2$ for $\varepsilon \to 0$
  - in the limit that the work function $\phi \approx 1/2(\phi_s + \phi_t) \gg eV_{bias}$, $\kappa \approx \frac{\sqrt{2m\phi}}{\hbar}$

1.3 Tersoff1985: Theory of the scanning tunneling microscope 10.1103/PhysRevB.31.805

- theory for tunneling between real surface and model probe tip- here the tip is modeled most simply as s-wave
- tunneling current proportional to local DOS at surface at the tip
- for tip of radius R and vacuum gap distance d, laterial resolution $\sim [2\text{Å}(R + d)]^{1/2}$; applied to 2x1 and 3x1 reconstructions of Au(110) and GaAs (110)
- in STM, height is adjusted to maintain same tunneling resistance between surface and tip –> contour map of surface
- analogy with planar tunneling, current decays with $\hbar(8m\phi)^{-1/2}$for ϕ work function
- surface treated "exactly" when tip is modeled as locally sphereical potential well (at the time, did not understand local geometry of the tip)
- STM relatively insensitive for position of surface layer relative to underlying layers (at least for Au)
- first-order PT (ish)

$$I = \frac{2\pi e}{\hbar} \sum_{\mu,\nu} f(E_\mu)([1 - f(E_\nu + eV)]|M_{\mu\nu}|^2 \delta(E_\mu - E_\nu)$$

V is applied voltage, $M_{\mu\nu}$is matrix element between $\psi_\mu$of the probe and $\psi_\nu$of the surface (which in general are nonorthogonal states of different Hamiltonians), $E_\mu$is energy of state $\psi_\mu$in the absence of tunneling

- since experiments are taken at small voltage and low temperature (i.e., ignore reverse tunneling) (in the context of metal surfaces- not sure for semiconductor)
- Bardeen showed that $M_{\mu\nu}$ is essentially the current operator

$$M_{\mu\nu} = \frac{\hbar^2}{2m} \int d\vec{S} \cdot (\psi_\mu^* \vec{\nabla} \psi_\nu - \psi_\nu \vec{\nabla} \psi_\mu^*)$$

where integral is over any surface lying entirely within the vacuum (barrier) region separating the probe and surface

- Surface wave function $\psi_\nu$is expanded as

$$\psi_\nu = \frac{1}{\Omega_s^{1/2}} \sum_G a_G \exp[\kappa^2 + |\vec{\kappa}_G|^2)^{1/2} \exp(i\vec{\kappa_G} \cdot \vec{x})$$

where $\kappa = \hbar^{-1}(2m\phi)^{1/2}$is the minimum inverse decay length for wave functions in vacuum; $\vec{\kappa}_G = \vec{k}_{||} + \vec{G}$ denotes surface Bloch and reciprocal-lattice vectors

- Probe wave function $\psi_\mu$is modeled as locally spherical potential well (assuming work function of tip is same as surface)

$$\psi_\mu = \frac{1}{\Omega_t^{1/2}} c_t \kappa R \frac{\exp(\kappa R)}{(\kappa|\vec{r} - \vec{r}_0|)\exp(\kappa|\vec{r} - \vec{r}_0|)}$$

- This (+ further assumptions and simplifications) leads to

$$M_{\mu\nu} = \frac{\hbar^2}{2m} \frac{4\pi}{\kappa \Omega_t^{1/2}} \kappa R \exp(\kappa R) \psi_\nu(\vec{r}_0)$$

where $\vec{r}_0$is the position of the center of curvature of the tip

- This leaves the final form for the tunneling current as

$$I = 32\pi^3 e^2 V \phi^2 D_t(E_F) \frac{R^2 e^{2\kappa R}}{\hbar \kappa^4} \sum_\nu |\psi_\nu(\vec{r}_o)|^2 \delta(E_\nu - E_F) \equiv 32\pi^3 e^2 V \phi^2 D_t(E_F) \frac{R^2 e^{2\kappa R}}{\hbar \kappa^4} \rho(\vec{r}_o, E)$$

where $D_t$is the DOS of the probe tip and $\rho(\vec{r}_o, E)$ is the surface LDOS

- spherical tip approx enters only in normalization of ψ_μ; this model less accurate for large R, where higher l becomes more important
- approximate methods for STM- STM provides limited information for smooth, low-Miller-index surfaces

- small voltages- tunneling from states near E_F- for semiconductors- n- and p-doping can give different STM images
- low doping or high voltages: voltage polarity may determing whether tunneling involves VBs or CBs (e.g,, Si (111) need large 2.5 V)
- GaAs(110) 1x1 reconstruction surface- got a qualitative difference of VBs and CBs

Numerical things to consider

- if the slab is too thiin- inaccurate work function; thin sparse sampling of bulk continuum leads to numerical noise in energy-projected quantities
- not good accuracy at distances far from surface
- limitations of plane-wave part in describing exponential decay inside deep troughs
- how many states from band edge to include in LDOS; within 1eV used for GaAS (110)

In summary, things that could lead to deviations from experiment

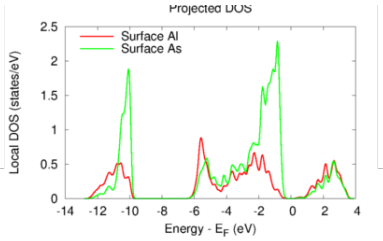
- tip geometry not properly taken into account (e.g., not have spherical potential well); s-wave treatment of tip without details of the geometry
- assumptions of tip radius and vacuum gap distance
- if can use similar assumptions of metal surface for which beginning is referenced to for a semiconducting surface
- if ϕ assumed same for tip and sample
- limits of validity of model
  - tip and surface do not have too large difference in work function- affects the effective $\kappa(\vec{r})$
  - implicit assumption that potential goes to zero in region between surface and tip- actually the electron is never more than 3-6 Ang from surface so magnitude of potential is never less than ~ 1 eV

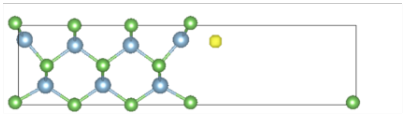
2 Practical calculation in QE

QE uses Tersoff-Hamann method.

2.1 AlAs(110) Tutorial (PP/examples/example03)

Here we chart out a workflow of generating the STM images for future reference, and to keep track of trains of thoughts. Generated from A free tool for flowcharts.





LDOS boxes (projwfc.x)

input	files	parameters
*box.projwfc.in	*box#i.xsf	tdosinboxes = .true. plotboxes = .true. n_proj_boxes = 8 *Defining boxes over atoms* *Based on FFT grid* irmin(i,j) irmax(i,j) where i = vector index j = box index *Normal DOS parameters* degauss DeltaE ngauss = 0

LDOS spectra projections (projwfc.x)

inputs	files	parameters
*projwfc.in	*pdos_atm#i(atom)_wfc*	tdosinboxes = .false degauss DeltaE ngauss = 0

scf & nscf run

dense kpt mesh

pp.x @ (positive) bias

input	files	parameters
*.pp_stm+.in	filplot/filepp= AlAsresm+1.0 fileout = AlAs110+1.0	plot_num = 5 (STM image) sample_bias (Ry) output_format = 2 (2D plotrho) *Define plane* e1(i) e2(i) x0(i) for i = 1,2,3 *Sampling* nx, ny

pp.x @ (positive) bias, constant current

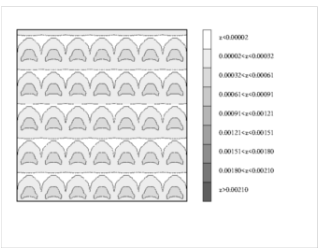
input	files	parameters
*.pp_isostm+.in	filplot/filepp= AlAsresm+1.0 fileout = AlAs110.pp_isostm+.dat	plot_num = 5 (STM image) sample_bias (Ry) output_format =7 (2D Gnuplot) *Define plane* e1(i) e2(i) x0(i) for i = 1,2,3 *Sampling* nx, ny *Constant Current* isostm_flag = .true. heightmin = 0.4 heightmax = 0.75 direction =1

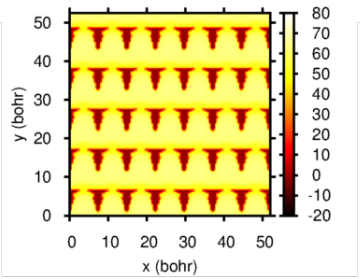
plotrho.x

input	parameters
*plotrho+.in	AlAsresm+1.0 (input file) Al110+1.0ev.ps (output file) logscale boolean rhomin, rhomax, nlevels

gnuplot

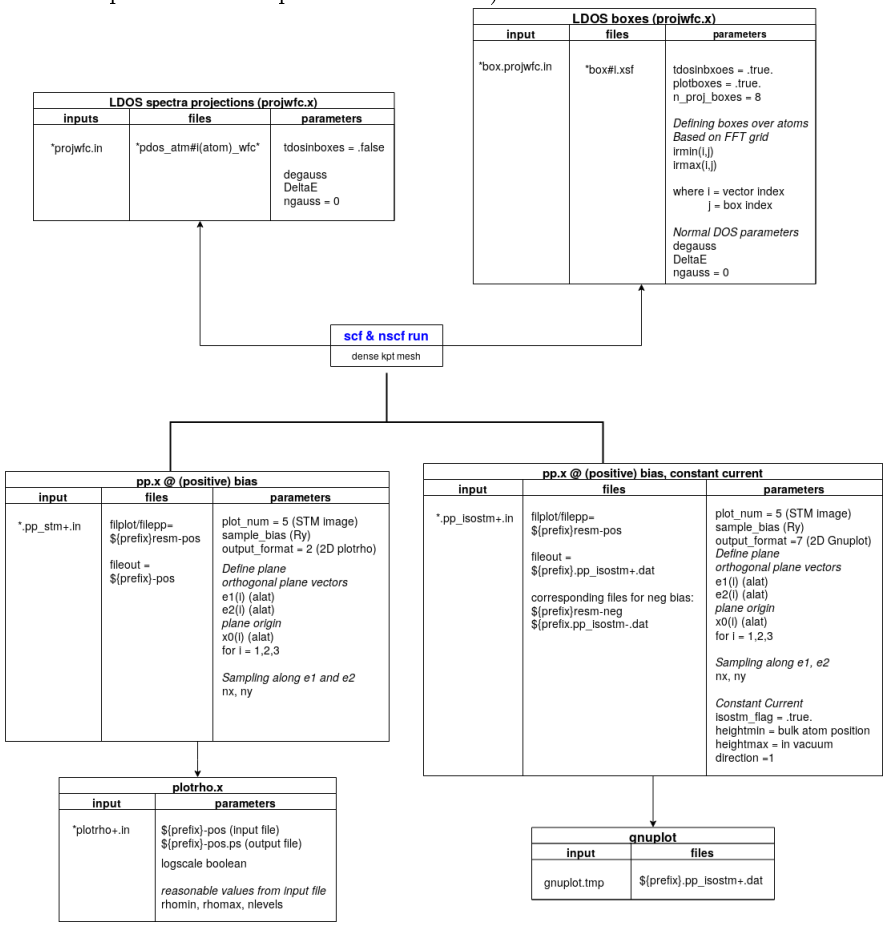
input	files
gnuplot.tmp	AlAs110.pp_isostm+.dat





2.2 Considerations for BiVO4

Adapted above workflow to generic run so that can just substitute multiple values. Separated generation of heat maps from LDOS plots (i.e., bottom half generated separate from top half of flowchart).



The following scripts are skeletons and may be adjusted based on user needs.
TODO: automatic choice for rhomin, rhomax for different biases

`stm_run.sh`

```
#!/usr/bin/env bash
# Adapted from PP/Example03
# Simulated STM image  # Generates STM image @ +/- bias
#                      @ +/- bias, constant current
#           Plot script for LDOS boxes
#           Plot script for LDOS spectra
# see below for environment variables: QEDIR, BIN_DIR, etc.
#   and change accordingly
# example usage
```

```
#    ./stm_run.sh
#    ./stm_run.sh stm_input.dat (default input file name)
#    ./stm_run.sh stm_AlAs.dat

### import input parameters
if [[ "$#" -eq 1 ]]; then
   input_file=$1
else
  input_file="stm_input.dat"
fi

# run from directory where this script is
cd `echo $0 | sed 's/\(.*\)\/.*/\1/'`  # extract pathname
EXAMPLE_DIR=`pwd`

# check whether echo has the -e option
if test "`echo -e`" = "-e" ; then ECHO=echo ; else ECHO="echo -e" ; fi

$ECHO
$ECHO "$EXAMPLE_DIR : starting"
$ECHO
$ECHO "Calculation of STM maps."

# these are default values, can be overridden
# adapted from environment_variables
QEDIR="/home/wwwennie/bin2/qe-6.3/"
BIN_DIR=$QEDIR/bin
PSEUDO_DIR=$QEDIR/pseudo
TMP_DIR=`pwd`
PARA_PREFIX=" "
PARA_PREFIX="mpirun -np 4"
PARA_POSTFIX=" -nk 1 -nd 1 -nb 1 -nt 1 "

# function to test the exit status of a job
check_failure () {
  # usage: check_failure $?
  if test $1 != 0
  then
     echo "Error condition encountered during test: exit status = $1"
     echo "Aborting"
     exit 1
  fi
}

prefix="pwscf"
source ./${input_file}
```

```
# required executables and pseudopotentials
BIN_LIST="pw.x pp.x plotrho.x projwfc.x sumpdos.x"
$ECHO
$ECHO "  executables directory: $BIN_DIR"
$ECHO "  pseudo directory:      $PSEUDO_DIR"
$ECHO "  temporary directory:   $TMP_DIR" $ECHO "  checking that needed directories and file

# check for directories
for DIR in "$BIN_DIR" "$PSEUDO_DIR" ; do
   if test ! -d $DIR ; then
       $ECHO
       $ECHO "ERROR: $DIR not existent or not a directory"
       $ECHO "Aborting"
       exit 1
  fi
done

for DIR in "$TMP_DIR" "$EXAMPLE_DIR/stm_results" ; do
  if test ! -d $DIR ; then
      mkdir $DIR
  fi
done
cd $EXAMPLE_DIR/stm_results

# check for executables
for FILE in $BIN_LIST ; do
  if test ! -x $BIN_DIR/$FILE ; then
     $ECHO
     $ECHO "ERROR: $BIN_DIR/$FILE not existent or not executable"
     $ECHO "Aborting"
     exit 1
  fi
done

# check for gnuplot
GP_COMMAND=`which gnuplot 2>/dev/null`
if [ "$GP_COMMAND" = "" ]; then
   $ECHO
   $ECHO "gnuplot not in PATH"
   $ECHO "Results will not be plotted"
fi
   $ECHO " done"

# how to run executables
PW_COMMAND="$PARA_PREFIX $BIN_DIR/pw.x $PARA_POSTFIX"
```

```
PP_COMMAND="$PARA_PREFIX $BIN_DIR/pp.x $PARA_POSTFIX"
PLOTRHO_COMMAND="$BIN_DIR/plotrho.x"
PROJWFC_COMMAND="$PARA_PREFIX $BIN_DIR/projwfc.x $PARA_POSTFIX"
SUMPDOS_COMMAND="$BIN_DIR/sumpdos.x"

$ECHO
$ECHO "  running pw.x as:      $PW_COMMAND"
$ECHO "  running pp.x as:      $PP_COMMAND"
$ECHO "  running plotrho.x as: $PLOTRHO_COMMAND"
$ECHO "  running projwfc.x as: $PROJWFC_COMMAND"
$ECHO "  running sumpdos.x as: $SUMPDOS_COMMAND"
$ECHO "  running gnuplot as:   $GP_COMMAND"
$ECHO

# post-processing for stm images (sample bias given in Ry!)
cat > ${prefix}.pp_stm-.in << EOF
&inputpp
  prefix  = '${prefix}'
  outdir='$TMP_DIR/',
  filplot = '${prefix}resm-neg'
  sample_bias=-${sample_bias_neg},
  plot_num= 5
/
&plot
  nfile=1
  filepp(1)='${prefix}resm-neg'
  weight(1)=1.0
  iflag=2
  output_format=2
  e1(1)=${e1[0]}, e1(2)=${e1[1]},     e1(3)=${e1[2]}
  e2(1)=${e2[0]}, e2(2)=${e2[1]},     e2(3)=${e2[2]}
  x0(1)=${x0[0]}, x0(2)=${x0[1]},   x0(3)=${x0[2]}
  nx=$nx ,ny=$ny
  fileout='${prefix}-neg'
/
EOF
$ECHO
$ECHO "  running the post-processing phase, negative bias...\c"
$PP_COMMAND < ${prefix}.pp_stm-.in > ${prefix}.pp_stm-.out
check_failure $?
$ECHO " done"

# run plotrho to do the figure
cat > ${prefix}.plotrho-.in << EOF
${prefix}-neg
${prefix}-neg.ps
```

```
n
${rhomin_neg} ${rhomax_neg}  ${nlevels}
EOF
$ECHO "  running plotrho on negative bias data...\c"
$PLOTRHO_COMMAND < ${prefix}.plotrho-.in > ${prefix}.plotrho-.out
check_failure $?
$ECHO " done"

# post-processing for stm images (negative bias, constant current)
cat > ${prefix}.pp_isostm-.in << EOF
&inputpp
/
&plot
  nfile=1
  filepp(1)='${prefix}resm-neg'
  weight(1)=1.0
  iflag=2
  output_format=7
  fileout='${prefix}.pp_isostm-.dat'
  e1(1)=${e1[0]}, e1(2)=${e1[1]},     e1(3)=${e1[2]}
  e2(1)=${e2[0]}, e2(2)=${e2[1]},     e2(3)=${e2[2]}
  nx=${nx_c}, ny=${ny_c}
  isostm_flag=.true.
  isovalue=${isovalue}
  heightmin=${heightmin}
  heightmax=${heightmax}
  direction=${direction}
/
EOF
$ECHO
$ECHO "  STM image, negative bias and constant current...\c"
$PP_COMMAND < ${prefix}.pp_isostm-.in > ${prefix}.pp_isostm-.out
check_failure $?
$ECHO " done"

# run gnuplot to do the figure
if [ "$GP_COMMAND" = "" ]; then
break
else
cat > gnuplot.tmp <<EOF
set term postscript enhanced color solid lw 3 24
set output '${prefix}-neg.isoplot.ps'
set xlabel "x (bohr)"
set ylabel "y (bohr)"
set pm3d map set size ratio -1
set palette rgb 21,22,23
```

```
set tics out
unset key
splot [0:51.972][0:52.500] '${prefix}.pp_isostm-.dat'
EOF
$ECHO
$ECHO "  plotting results ...\c" $GP_COMMAND < gnuplot.tmp
$ECHO " done"
rm gnuplot.tmp
fi

# post-processing for stm images (as before, but positive bias)
cat > ${prefix}.pp_stm+.in << EOF
&inputpp
  prefix  = '${prefix}'
  outdir='$TMP_DIR/',
  filplot = '${prefix}resm-pos'
  sample_bias=${sample_bias_pos},
  plot_num= 5
/
&plot
  nfile=1
  filepp(1)='${prefix}resm-pos'
  weight(1)=1.0
  iflag=2
  output_format=2
  e1(1)=${e1[0]}, e1(2)=${e1[1]},     e1(3)=${e1[2]}
  e2(1)=${e2[0]}, e2(2)=${e2[1]},     e2(3)=${e2[2]}
  x0(1)=${x0[0]}, x0(2)=${x0[1]},   x0(3)=${x0[2]}
  nx=$nx ,ny=$ny
  fileout='${prefix}-pos'
/
EOF
$ECHO "  running the post-processing phase, positive bias...\c"
$PP_COMMAND < ${prefix}.pp_stm+.in > ${prefix}.pp_stm+.out
check_failure $?
$ECHO " done"

# plotrho
cat > ${prefix}.plotrho+.in << EOF
${prefix}-pos
${prefix}-pos.ps
n
${rhomin_pos} ${rhomax_pos} ${nlevels}
EOF
$ECHO "  running plotrho on positive bias data...\c"
$PLOTRHO_COMMAND < ${prefix}.plotrho+.in > ${prefix}.plotrho+.out
```

```
check_failure $?
$ECHO " done"

# post-processing for stm images (positive bias, constant current)
cat > ${prefix}.pp_isostm+.in << EOF
&inputpp
/
&plot
  nfile=1
  filepp(1)='${prefix}resm-pos'
  weight(1)=1.0
  iflag=2
  output_format=7
  fileout='${prefix}.pp_isostm+.dat'
  e1(1)=${e1[0]}, e1(2)=${e1[1]},     e1(3)=${e1[2]}
  e2(1)=${e2[0]}, e2(2)=${e2[1]},     e2(3)=${e2[2]}
  nx=${nx_c} ,ny=${ny_c}
  isostm_flag=.true.
  isovalue=${isovalue}
  heightmin=${heightmin}
  heightmax=${heightmax}
  direction=${direction}
/
EOF
$ECHO
$ECHO "  STM image, positive bias and constant current...\c"
$PP_COMMAND < ${prefix}.pp_isostm+.in > ${prefix}.pp_isostm+.out
check_failure $?
$ECHO " done"

# run gnuplot to do the figure
if [ "$GP_COMMAND" = "" ]; then
break
else
cat > gnuplot.tmp <<EOF
set term postscript enhanced color solid lw 3 24
set output '${prefix}-pos.isoplot.ps'
set xlabel "x (bohr)"
set ylabel "y (bohr)"
set pm3d map set size ratio -1
set palette rgb 21,22,23
set tics out
unset key
splot [0:51.972][0:52.500]
'${prefix}.pp_isostm+.dat'
EOF
```

```
$ECHO
$ECHO "  plotting results ...\c" $GP_COMMAND < gnuplot.tmp
$ECHO " done"
rm gnuplot.tmp
fi

# Projection of the DOS on volumes (boxes)
cat > tmp.box.projwfc.in << EOF
&projwfc
  prefix  = '${prefix}'
  outdir='$TMP_DIR/',
  ngauss=0
  degauss=${degauss}
  DeltaE=${DeltaE}
  tdosinboxes=.true.
  plotboxes=.true.
  n_proj_boxes=${n_proj_boxes}
/
EOF
$ECHO
cat tmp.box.projwfc.in $TMP_DIR/tmp_box > ${prefix}.box.projwfc.in
$ECHO "  running local DOS calculation...\c"
$PROJWFC_COMMAND < ${prefix}.box.projwfc.in > ${prefix}.box.projwfc.out
check_failure $?
$ECHO " done"

# Projection of the DOS on atomic wavefunctions
cat > ${prefix}.projwfc.in << EOF
&projwfc
  prefix  = '${prefix}'
  outdir='$TMP_DIR/',
  ngauss=0
  degauss=${degauss}
  DeltaE=${DeltaE}
  tdosinboxes=.false.
/
EOF
$ECHO
$ECHO "  running projected DOS calculation...\c"
$PROJWFC_COMMAND < ${prefix}.projwfc.in > ${prefix}.projwfc.out
check_failure $?
$ECHO " done"
$ECHO
```

Uses the data file `stm_BVO.dat`

```
#!/bin/sh
# input file for stm_run.sh

prefix="66-s25v20"
# sample_bias defines energy window from E_fermi
# neg -> VB; pos -> CB (check this)
sample_bias_neg=0.29399d0
sample_bias_pos=${sample_bias_neg} # Ry

# pp
# plotting plane vectors and origin
# in units of alat; generates plot with repeated cells
e1=(7.0 0.0 0.0)
e2=(0.0 7.0 0.0)
x0=(0.0 -0.0 1.6742) # somewhere in bulk, on atom slice
nx=36 ny=56

# plotrho
# stm @ bias
# choose rho* from ${prefix}-neg or ${prefix}-pos
rhomin_neg=0.00000006
rhomax_neg=0.0000003
rhomin_pos=${rhomin_neg}
rhomax_pos=${rhomax_neg}
nlevels=8

# stm @ bias, constant current nx_c=150 ny_c=150 isovalue=1e-6
# height*=[0,1], % wrt cell height
# put heighmin somewhere in bulk, heightmax somewhere in vacuum
heightmin=0.7
heightmax=0.9
direction=1 # +/- 1

# LDOS boxes
degauss=0.001
DeltaE=0.002
n_proj_boxes=8

# sum pdos atom list
pdos_atoms=("Bi" "V")
eFermi=4.2  # eV, approx from nscf_10

# cat for boxes; based on FFT grid spacing
# at 90 Ry, BVO FFT = (60 60 675)
# surf1 @ 0.78
# surf2 @ 0.21
```

```
vac1_min=575
vac1_max=590
vac2_min=100
vac2_max=110
cat > tmp_box << EOF
!! Boxes centered on the first vacuum layer:
  !! 1) above the surface V
   irmin(1,1)= 0, irmax(1,1)= 4, irmin(2,1)= 5, irmax(2,1)= 20, irmin(3,1)=${vac1_min}, irma
  !! 2) above surface Bi
   irmin(1,2)=25, irmax(1,2)=35, irmin(2,2)= 5, irmax(2,2)= 20, irmin(3,2)=${vac1_min}, irma
  !! 3) across surface V
   irmin(1,3)= 1, irmax(1,3)=25, irmin(2,3)=1, irmax(2,3)=60, irmin(3,3)=${vac1_min}, irmax(
  !! 4) across surface Bi -> V
   irmin(1,4)= 1, irmax(1,4)=60, irmin(2,4)= 1, irmax(2,4)=25, irmin(3,4)=${vac1_min}, irmax

!! Same as above, centered on the second vacuum layer:
  irmin(1,5)= 0, irmax(1,5)= 4, irmin(2,5)= 5, irmax(2,5)= 20, irmin(3,5)=${vac2_min}, irmax
  irmin(1,6)=25, irmax(1,6)=35, irmin(2,6)= 5, irmax(2,6)= 20, irmin(3,6)=${vac2_min}, irmax
  irmin(1,7)= 1, irmax(1,7)=25, irmin(2,7)=1, irmax(2,7)=60, irmin(3,7)=${vac2_min}, irmax(3
  irmin(1,8)= 1, irmax(1,8)=60, irmin(2,8)= 1, irmax(2,8)=25, irmin(3,8)=${vac2_min}, irmax(
/
EOF

# running parameters
# see stm_run.sh for full list
PREFIX="/home/wwwennie/bin2/qe-6.3"
PSEUDO_DIR=$PREFIX/pseudo
PARA_PREFIX="mpirun -np 48"
PARA_POSTFIX=" -nk 4 -nd 4 -nb 1 -nt 1 "
```

3 Potentially useful tools

Oxygen octahedra picker: A software tool to extract quantitative information from STEM images; 10.1016/j.ultramic.2016.06.001