Hive:
STM images from VASP

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Dear user,

This file contains a quick introduction to the STM program: Hive (for VASP).

I) Installation

The installation of the program is quite straight forward. Simply unzip the windows-executable to the location of your choice, and start running the program.
Note: *It might be necessary to install an additional dll-file (**qtinf70.dll**) which is either supplied or can be found easily(and free) on the web.*

II) Conditions for code usage:

- If you like the results and use figures generated with the program in one of your articles, acknowledgement should be done by referral to this paper:
  Formation of Pt-induced Ge atomic nanowires on Pt/Ge(001): A density functional theory study -- **Danny E.P. Vanpoucke and Geert Brocks**
  Phys. Rev. B **77**, 241308(R) (2008)
  link to article

- If you encounter a bug/error/… please inform me of this trough e-mail: d.e.p.vanpoucke@tnw.utwente.nl or dannyvanpoucke@hotmail.com
- You are not allowed to distribute the program or claim it your (programming-)work.
- You run the program at your own risk, any possible damage to your machine, or mental health of you or your pets are your responsibility ☺

(**optional**;-))If you use the results in a paper, just for my personal curiosity I would be interested in a link to that paper, just to see what people are using the program for.

III) Creating VASP input for the Hive program:

For this I mainly refer you to the VASP manual:
http://cms.mpi.univie.ac.at/vasp/vasp/vasp.html
more specific to the topic of band decomposed chargedensity:
http://cms.mpi.univie.ac.at/vasp/vasp/node154.html

Typically you will have to do a selfconsistent calculation, which outputs a WAVECAR file, this WAVECAR file is then used to generate the partial charge densities. So make sure that in the run of the partial charge density calculation you find a line telling you explicitly that the WAVECAR was read successfully. Calculations for partial chargedensities are are very fast(compared to your other calculations) but they still need the same amount of memory as the selfconsistent calculation. So the easiest way of working is using a script which first does a selfconsistent calculation and then copies the WAVECAR, POTCAR, and POSCAR, and generates the needed INCAR and then runs a few partial charge density calculations.(don't forget to save your output of each run separately ☺.

Typical additional input for the INCAR file for a partial charge density calculation is:

Band decomposed Chargedensity:

```
    LPARD = .TRUE.   ! calculate Band decomposed chargecars(PARCHG)
    NBMOD =  -3      ! Calculate partial charges for e- with eigenvalues in interval EINT to
                     !  Fermi level
    EINT  = -1.50    ! from 1.5eV below Fermi level to Fermi level
```

Extra options such that VASP has no excuse to fail

```
    ISTART = 1           ! explicitly tell to use old WAVECAR file
    NBANDS = $NBDS  ! different amount of cpus = different amount of bands = VASP
```

refuses to use WAVECAR and sets up a random one➔ so you need to read the number of bands from your selfconsistent calculation. This can be done with a commandline like this: NBDS=`grep NBANDS OUTCAR |awk '{print $9}'`, if you then write the INCAR for the partial charge density calculations in a script you can use $NBDS as input(like I do here), or you can put the number there manually.

IV) Small Manual for the Hive program:

The only thing you need is a CHGCAR or PARCHG file,

1) You load it with the button “Load PARCHG file”.
2) Select the orientation of the slab
3) Select the direction of the tip, are you looking down(towards 0) from the center of the cell or up(towards 1)
4) Select either the Constant Charge Density (CCD) level (in vasp units) or Distance to highest atom (in Angstrom). If you use the later one, the program will show you the CCD value at that height(it does not work the other way around)
5) Run STM, to see a grayscale STM image.
6) You can show the atom locations which are within the thickness-range of your STM surface (If you see nothing appear it means that the lowest position (black in the grayscale image)) of your isosurface is still above the highest atom.
7) Contours can also be added to guide the eye, enter a number for the upper and lower boundaries of the contour interval, and select a number of contours you want to draw. Please stay within the range of the STM grayscale, i.e. min>=0 and max<= value at the top of the grayscale-scalebar at the right of the image)
8) Contours and atoms are drawn when you press “run STM”, but it is faster to update them through “Draw overlay” or “erase overlay”
9) Clicking at a position in the STM image will give you some information about that location: its coordinates, the “height” of the isosurface at that point, and the height of the atom (in the isosurface scale) if one is present.
10) The options underneath are save-options for an inputfile of a 3D program I’m working on, so you van ignore those.
11) Saving your STM image: go to the menu STM-options and select “save image”, the image you have on screen will be saved to a bmp. Save atomposImage can be used to save only the overlay
12) The averaging tool on the second tab, just give you the average of the area you select on the STM image, and a primitive distribution is drawn on the tab “distribution plots” They can be ignored as should be the tabs “geometry”.

V) Tools-section:

Under the Tools-tab some extra useful options are hidden.

1. **Tools off**: neither the linescan tool nor the averaging tool can be used
2. **Averaging tool**: can be used to find the average "height" in either a rectangular of ellipsoidal area. Click on the STM image to place the rectangle/ellipse where you like. Press the button "Find average" for the average inside the red rectangle/ellipse to be shown. A distribution of the heights present are also very crudely plotted under the tab: "distribution plots". No save option exists.
3. **Linescan tool**: can be used to generate a linescan over your STM image. Select the begin (right click) and end (left click) points of your scanline and hit the "make linescan" button. A linescan image will be drawn on the "distribution plots"-tab. The image shown there is only a rough sketch, you can save the dataset however via the "Tool options" menu. The output consists of 2 columns containing the (r,z) coordinates of the linescan and can be plotted using your favorite plotting software. (units for r and z are Angstrom)

The **grayscale scale option** is mainly for those more advanced users who want to manually define the range of the grayscale of the calculated STM images. Either to compare different systems as if they would be plotted in the same grayscale, or to limit the STM depth if one for example works with a 1D system.
In case of the latter the STM will move trough the entire cell when it is positioned next to the 1D object (this is shown by the bright pink in the STM image). One drawback in this situation is that the range of the grayscale will grow to be the full(or half full) height of your cell, losing any contrast on the 1D object. With this option one could reduce the range to for example only the top 1.5A of the STM image, spread the entire grayscale over this 1.5A, and make everything below black.
One small remark here: be careful when plotting contour-plots on such STM images, make sure that the limits of the contour plot are within the specified range you have given.

VI) Q&A

- In what units is the Constant Charge Density (CCD) level given?
  - In electron per cubic angstrom (e/A^3)

- I see pink in some of my images, pink isn't a grayscale, is it?
  - I used fuchsia (a.k.a. RGB=#FF00FF) to identify the places where the STM tip moves trough the entire height of the cell without ever meeting it's "constant current" surface. This can happen if you have chosen the CCD level to large, or the distance to the highest atom (z) value to small such that you have to go to close to the atom cores. In that case holes appear between your atoms. Also 1D systems could show this in the region next to the 1D object. In case of the first change your CCD/z level to something more reasonable, for the later I suggest to use the Grayscale scale option in the "tools"-tab.

- I noticed the CCD value changing when I change the z value and run the STM(and vice versa. What is going on?
  - Each CCD value can be transformed into a specific z value (which depends on your system). The program does this for you. This allows for better comparison between different systems. If for the first system you chose a hight to highest atom z=3.0A, then using the obtained CCD value you can make a pseudo STM image of a different system showing the same isosurface. In combination with the Grayscale scale option in the "tools"-tab even the grayscales can be matched.

- Do I need to rerun the STM to draw contours or atom positions?
  - No, you don't. You can instantaneously add and remove them using the Draw/Erase Overlay buttons.

- I notice some options for saving the STM images as a 3D-image, how can I use them?
  - The 3D program written for this is not publicly available (yet). But the formatting of the output is quite straightforward, so you could easily write your own 3D plotter to read those files and generate images from them.

VII) Troubleshooting: Some warnings about the program.

- The program is a purely windows program (so it won't work under Linux, etc…), written in Delphi. There is a chance that when you run the program it will complain that a certain dll is missing, this dll can be found easily on the internet and should solve this problem(sorry for the inconvenience).Most probably it will be the ***qtinf70.dll*** .(which should be included)
- Since the program is written with my own specific problem in mind there are some things you should take into account:
    - The center of your (super)cell should be the center of your vacuum layer, so your structure is best to be centered around the 0 plane(in the direction orthogonal to your surface)
    - If you use a dipole correction there might be problems, because the "STM tip" should start in the center of the cell, which should be the center of the vacuum. (this is a problem on my to-do list to solve)
    - The approximation for the tip is a point source(i.e. there is no actual tip geometry involved→ cf. Tersoff-Hamann paper for more information.)
      → the consequence of this approximation is that you will obtain very sharp STM images with a resolution not obtainable by real-life STM, this has the advantage that you see features very clearly, making it easier to recognize them in experimental STM image.
      To-do: add a simple smoothing function to simulate tip width

Now you know all there is to know about how to use the program. Enjoy.

Kind Regards,
Danny Vanpoucke
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