

Installation instructions

1. Download

Get the right binary for your machine

from <https://www.scm.com/support/downloads/> using your userid and password for the course

2. Install

- a. Windows: run the exe with Administrator privileges, accepting all defaults.
- b. Mac: open the dmg and drag the AMS2023.xxx item to the Applications directory.
- c. Linux desktop: follow the instructions in the Linux Quick Start guide: https://www.scm.com/doc/Installation/Linux_Quickstart_Guide.html

3. Run

- a. Windows: double-click the AMSjobs shortcut
- b. Mac: run the AMS2023.xxx application
- c. Linux: set up your environment, run \$AMSBIN/amsjobs

You will be prompted for your username, password, and email address when you first use AMS.

After submitting your (correct) details, a license will then automatically be retrieved and installed.

This license will allow you to run the purchased AMS modules.

If you do not succeed, you can check our instruction videos about installation of AMS at <https://www.scm.com/support/ams-installation-videos/>

If you get a license error please send the error message to license@scm.com.

Your first band structure

1. Open AMS2023, then click **SCM** → **new input**.
2. A new window opens, where you can build molecules and structures, and where you can even run (simple) molecular dynamics simulations. In the default setting on Apple, a **machine-learning (ML) potential, ani-1ccx** is used. In Windows, this is a simpler force field model (it can be changed by **AMSinput** → **Preferences** → **Pre-optimizer**, for more: GUI manual with link on next page). Click on **C** in the bottom of the window, which represents a carbon molecule, and click anywhere to place a carbon. Draw a sloppy hexagon, adding 5 more carbons this way. Press **escape** to stop adding carbons. Then, click on the wheel-like button on the very right. It may take a little initialization to optimize, but then it works very fast. You can check the bond lengths by selecting two elements, while holding **shift** (doing the same with three gives you an angle).
3. However, we are not interested in molecules, but in solids. To move to the periodic version of the software, click on the dark-yellow **ADF** button, and select **BAND**. We are going to build a chain of hydrogens. Just put a single hydrogen (**H**) anywhere; press **escape** after placing one atom in the window.
4. We are going to put this single hydrogen atom at 0,0,0 in our Cartesian coordinate system. Do this by **model** → **coordinates**. There, manually, **set H(1) at 0,0,0**.
5. Now, move to **model** → **lattice**. Here, we will specify what sort of crystal structure we want. We will build a chain of hydrogens, so select **Periodicity: chain**. Only one value can be entered there, which is the distance between hydrogens in the chain. Put 1.0, for a 1.0 Å spacing. Nothing happens in the main window, but this is because in many lattices, a periodic display becomes visually intractable. Click on the square of four circles (three white, one black) to turn on periodic display. Now, a few H's (a few unit cells) are shown. Right-click on the same button to choose a larger range of unit cells to display, if you wish.
6. Move to **Main** and select **Calculate band structure**. Save your project, under whatever, then do **File** → **Run**. You will see your quantum-chemical calculation progressing in the AMSjob window. It should be very fast.

- When the calculation is finished, go **SCM → Band structure**. You will see your (likely first) band structure, the one of a chain of hydrogens, which we will discuss in class. On the right, you can see a 'Density-of-states'. Try to see if you can spot a (simple) mathematical relationship between the two.

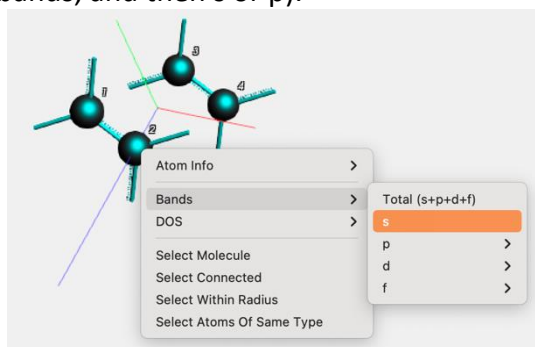
Manuals

GUI: <https://www.scm.com/doc/GUI/index.html>

BAND: <https://www.scm.com/doc/BAND/index.html>

Exercise 1: C-C and B-N

- By nature of their elements, what do C-C and B-N have in common?
- On materialsproject.com, find the crystal structure of graphite (mp-48), carbon (C) in a hexagonal structure of $P6_3/mmc$ symmetry, and download its .cif file. Open the file with AMS, calculate the band structure, and base a brief characterization of the material on that.
- Visualize the contributions of C, the 2s orbital, and the 2p orbitals (select all atoms, right-click, select bands, and then s or p).

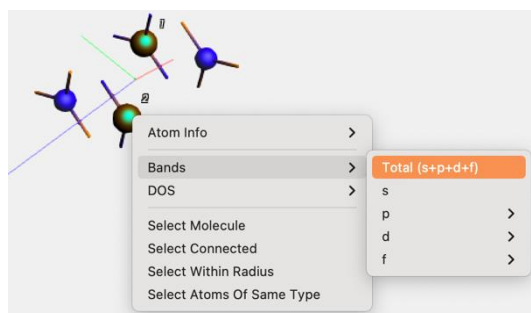


You might need to zoom out to see the 2s.

Save the project for later

- Find the crystal structure of boron nitride (BN, mp-984) on the materialsproject, download the .cif file, and calculate the band structure. What are the differences with graphite?

5. Visualize the different contributions of the B and N orbitals to the band structure.



From C-C to B-N, we have introduced (a degree of) ionicity. How is this reflected in the band structure?

6. Reopen the C-C project. Rotate, and delete the two bottom C's. Then move to **Model**, and change **Periodicity** from **Bulk** to **Slab**. You have just created graphene. Save as a separate project, and run a band structure calculation. What do you see?
7. Do the same, but now for B-N. Plot the band structure of this 2D B-N, and describe what you see.
8. By going from C-C to B-N, we introduce ionicity, but (and this is particularly well visible for the 2D systems) we change one other fundamental property: symmetry. Can you give a description of how symmetry has changed. If you know Group Theory, you can use Point Groups. If you don't, think of rotation axes.
9. Download the .cif file of diamond (C, mp-66) another form of carbon. Plot the band structure. Describe the symmetry and bonding.

Homework

You have now seen, in class, how bonding and symmetry affect the electronic structure, and may set a band gap. The band gap is very important in photovoltaics, because it determines the wavelength at which light is absorbed. For absorption of solar light, we need a semiconductor with a gap, roughly between 1.1 and 1.5 eV.

The following exercise is group work, and consists of two parts. Let two members of your group present the results on Monday, in class. The tasks are:

- 1- Find the diamond-type structures of Si (group 1), Ge (group 2), GaP (group 3) and CdTe (group 4). For help on finding the structures on materialsproject: diamond-type structures are cubic and have a two-atom basis. Provide a description of the band structure, and compare the band gap and chemical bonding to that of diamond.
- 2- On the materialsproject, find a material with a band gap between 1.1 eV and 1.5 eV. Plot the band structure, describe the bonding, and if possible, how that connects to the observed band gap.