Group Handbook

A guide to help you start your scientific adventures

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hackingmaterials.lbl.gov

maintained by Anubhav Jain

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Preamble

Welcome to the HackingMaterials research group! The purpose of this guide is to ease your transition into our research group and help make your time here as productive and enjoyable as possible.

An editable copy of this guide is always available at:
https://bit.ly/2huxUJW

Anyone (including those not in the group) can comment freely there - please submit suggestions, improvements, and corrections! You can also download the latest "PDF release" of this guide at
https://hackingmaterials.lbl.gov/handbook.pdf

We thank Valve software (a video game company) for openly publishing their employee handbook. Their guide helped inspire this effort.

Finally, thank you to those who help create and update this guide; each of us gains from the contributions of those before us, and we hope you are able to pay it forward to future members by contributing as well.

About our group

Our group is located at Lawrence Berkeley National Laboratory (LBNL) in Berkeley, California. LBNL is managed by the University of California at Berkeley, which is located just down the hill. 13 Nobel prizes have been awarded to scientists from LBNL. The lab has spectacular views of San Francisco, which is located across the bay and is about a 30 minute drive or BART train ride away. Berkeley itself is a vibrant city of 115,000 people filled with cafes, restaurants of all types, and cultural activities.

Our group aims to tackle some the most important problems lying at the intersection of materials science and computer science. We differ from a traditional materials theory group in our emphasis on building long-term software, in leveraging large supercomputers, and in applying statistical learning to materials problems. Most of our projects use a "materials genomics" approach, a new mode of research that has tremendous potential to discover new materials and to improve our fundamental understanding of how materials behave.

Our research group is its own microcosm within the materials science theory efforts at Berkeley. In the same way that Berkeley is a small city adjacent to the bigger city of San Francisco, our group is a smaller unit

linked to the larger theory groups of Kristin Persson, Gerbrand Ceder, Jeffrey Neaton, and Mark Asta – creating a close-knit community of materials theory within Berkeley. We also collaborator with groups external to the Berkeley area, and thus it is almost always the case that *someone* within our collaboration circle has experience with any new methods or applications you might be interested in. We hope you are able to leverage many of these resources during your stay!

Many new discoveries remain to be uncovered in the field of materials design and in our relatively new subfield of materials informatics. Your contributions are urgently needed to make this new vision a reality - welcome!

Before you arrive

Although many things can only be taken care of after arriving at LBNL, here are a few simple things you should do in advance.

Join the Slack group!

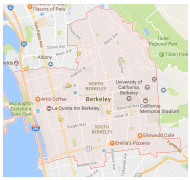
The berkeleytheory Slack group spans several research groups at LBNL. There are channels to ask housing questions, programming questions, science discussion, and general hijinx.

How? **Contact Anubhav - he'll introduce you.**

Order a computer!

Postdocs and graduate students - let's order your workstation in advance so that it's ready by the time you arrive.

How? **See Appendix on purchasing a computer.**



Find a place to live!

Berkeley and the surrounding areas are wonderful places to live, but finding an apartment can be difficult and is best done with knowledge of the various neighborhoods.

How? **See Appendix on housing.**

After arriving at LBNL

Welcome to Berkeley! Here are a few pointers for getting started.

Getting set up to work

Here is a short checklist of things you should do sooner rather than later:

- ❑ **Set up your computer**. See Appendix documentation on how to do this and some recommended software to install.
- ❑ **Complete the checklist that HR gives you in your welcome package.** Note: postdocs cannot select retirement plans. If you are a postdoc, you do not need to do anything and disregard the documents HR gives you on different retirement plans; an obligatory UCRS DCP is deducted from your pre-tax salary each month but the money belongs to you.
- ❑ **Complete all LBNL training courses.**
- ❑ **Set up the employee wifi**. Note that the visitor wifi is open access. To connect to employee wifi, go to ***https://software.lbl.gov/***, search for "Wireless Networking", and download the configuration file.
- ❑ **Install VPN for connecting to the lab network from home.** For example, this lets you download research articles from home. See ***https://software.lbl.gov*** for instructions on installation.
- ❑ **Obtain user accounts for any computing resources you may be using**. See further documentation later in this handbook.

- ❑ **Obtain a license for any software packages you might be using.** For example, you may need to be added to the VASP users list (for VASP, you should also register for the forum.)
- ❑ **Set up the printer.** It should appear on your network as "Toshiba e-studio" and you should be able to connect if you are on the LBNL network (e.g., if you are using an ethernet cable). The printer is located in the corner of the third floor of building 62 near the water fountain.
- ❑ **Request after-hours access**. By default, you will not have off-hours site access to building 62, *i.e.*, on weekends, holidays, and from ~6pm to 7am on weekdays. To obtain off-hours site access, email the Site access office at the lab (*siteaccess@lbl.gov*) and cc Anubhav.
- ❑ **Have your picture taken for the group web site.** Coordinate this with Anubhav, who will take the picture.
- ❑ **Say "hi" to your neighbors!** Working here will be more pleasant if you get to know some of the people around you, including those that work in other research groups.

Getting situated in your office

There is no rule that says your office must be dull and generic. Decorate your lab space with photos, posters, or other personal touches. You are likely going to be sitting in this office for quite some time so you should take a moment to make this space your own.

Food and coffee

There is a common kitchen in building 62 with microwave, mini-fridge, and coffee machine. I don't know who the coffee machine belongs to but

you can try to make friends with whomever that is. For *emergency* coffee situations, Anubhav has an espresso machine in his office that you can borrow (but wait for the go-ahead to come in, since he is often in the middle of a videoconference).

There are no vending machines in building 62, but if you go down to the first floor you walk to building 66 and there are some vending machines on the bottom floor. There are also some vending machines on the bottom floor of 67 (Molecular Foundry).

The only real food is in the lab cafe, which is about a 15 minute walk from our building. The menu is posted at (some items change weekly): ***http://www.bayviewcafelbl.com***

Mail

The incoming and outgoing mail corridor is located in building 62, second floor. You can find an empty slot and put your name there; sometimes, your mail will end up there, other times your mail will just end up in a common pile, so you may need to check both. Please do not have any personal (non-business related) mail sent to your LBNL address - this is not allowed.

If you would like to mail something internally (including the benefit office, which is not on the hill), get a special envelope from building 66, scratch off all the previous mail stops and write down the destination mail stop (something like: 90P-0101) and then put it in the outgoing mailbox in the mail corridor in 62.

Equipment and conference rooms

Should you need it, Anubhav has a projector that you can borrow. If he is not in the office, feel free to go in and just grab it (it is visible on the gray shelf). Just leave a note and remember to return it.

Anyone can reserve conference rooms through the LBNL Google calendar. Make sure you are logged in to your lbl.gov account.To see the availability of a room, just add the conference room calendar to your list of calendars (find the area that says "Other calendars" and then type the room into "Add coworker's calendar"). To book a room, add an event to your own Google Calendar and use the option within Google calendar to add a room. You will see a list of LBNL rooms displayed. *e.g.*, 62-203 (big main room) and 62-253 (smaller room with poor wi-fi). Note that when adding a room, you will see a number in parenthesis like (20) - that is approximately the number of people that the room can accommodate. For more detailed information, see ***https://commons.lbl.gov/display/fac/Conference+Rooms***.

The Panic Monster

The Panic Monster is a red doll in Anubhav's office based on a blog post from *Wait But Why*. If you see the Panic Monster on Anubhav's desk, it is best not to bother him. If you see the Panic Monster on *your* desk, it means you have lots of work to catch up on and you need to get working!

What to do if you're sick

If you're sick, ***do not come to the office***. This is very important; otherwise, you can get others sick and potentially bring down the productivity of the entire group. Instead, work from home or take a sick day to rest, relax, and recover. Simply e-mail Anubhav and let him know what you're doing. Just don't come into the office!

Other issues

If you are struggling with stress or other personal problems, you can contact the LBNL Employee Assistance Program (EAP), which provides free and confidential counseling, consultation, and referral for LBNL staff. If you are comfortable doing so, you can also discuss the problem with me and we can discuss if there are ways forward.

Making purchases

You are encouraged to make purchases that are likely to save you a lot of time. For example, if a commercial version of a software is superior to open-source alternatives, then you should purchase the commercial version. Your time is valuable and if we can solve a problem with funds, then we should try to do so.

Purchases are usually paid for through **project ids** that Anubhav can provide you with. For items less than $100, you should initiate purchases on your own provided that you know the correct project id. For items greater than $100, contact Anubhav first.

The procedure for making purchases depends on the purchase type:

- **Software**: Many popular commercial software libraries (e.g., Microsoft Office) can be purchased through *software.lbl.gov*.
- **Office supplies, computer accessories**: Check the LBNL's Ebuy (*not* Ebay) first via *procurement.lbl.gov*. If the item or an equivalent is available, this is the easiest way to make the purchase (for both you and LBNL administration)
- **Other purchases:** You should coordinate other purchases with the division's administrative contacts (currently esdradmin@lbl.gov). Most likely, someone will ask you to fill out a simple purchase order.

Booking conference travel

Graduate students and postdocs are encouraged to attend conferences for professional development and to broadcast your work to the research community. Many if not most people learn about new research by hearing about it at a conference. Thus, if you want people to know about your work, you must be willing to tell people about it. Anubhav encourages you to be proactive in seeking out conferences that may be beneficial for you to participate in.

You should identify conferences you'd like to attend several months (usually ~4 months, perhaps ~6 months for international travel) in advance. Usually, this is around the same time that abstract deadlines are due.

Once you have identified a conference you'd like to attend, please take the following actions:

- Tell Anubhav about the conference and what project you'd like to present
- Work with Anubhav to submit an abstract
- As soon as possible - submit a conference travel request form. This form is a very basic (i.e., 2 minutes to fill out) Google spreadsheet and usually there is an email with a link to it sent out every few months.. If you don't have it, then email esdradmin@lbl.gov to obtain it. If you do not submit the travel request form several months in advance, you may not receive LBNL approval to attend.
- If you haven't done so already, make sure your travel profile (*e.g.,* your frequent flier programs) are completed for the lab. E-mail Charlotte Standish if you don't have one yet.

Once you have received approval to attend the conference, please take the following steps:

- Make sure you register for the conference in time to receive any early registration discount *(normally on one's own credit card then reimbursed later)*
- Book a hotel *(normally on one's own credit card then reimbursed later)*
- Book a flight - please do this early to avoid last-minute flight rate spikes *(normally booked in coordination with Charlotte Standish with LBNL making the booking. This works better if you identify desired flights in advance, otherwise give Charlotte the preferred dates and times.)*
- If you are planning to combine vacation and travel, remember the lab's policy of taking only one vacation day per two work days. Note that days spent traveling to and from the conference count as work days.

In terms of travel receipts and reimbursement:

- If you are traveling with funding through LBNL (i.e., most cases), you do ***not*** need to save receipts for meals. You will receive a per diem instead. You also do not need receipts for taxi rides under $75, although Anubhav usually submits them anyway when he has them. You also do not need to save your actual airplane tickets for lab-purchased airfare, although again Anubhav usually submits these anyway.
- If you are traveling with outside funding (e.g., the conference organizers are going to reimburse you), save all receipts and tickets as they may be needed for reimbursement.
- When returning from travel, coordinate reimbursements with Charlotte Standish. You can also ask Charlotte about any travel questions that might not be covered here.

Asking your advisor for research help

From time to time, you will encounter problems, require suggestions, or otherwise need assistance from your advisor. This is normal, and asking for help is encouraged so long as you have done your best to solve the problem yourself. Sadly, it is all too easy these days to send e-mails without first investigating a problem yourself, and it is important to remember that your advisor gets many dozens of emails per day. Thus, if the question is important and difficult enough to ask your advisor, you should take the time to address the following four questions[1]:

[1] These guidelines are adapted from Dale Carnegie.

❑ **What is the problem?**

Clearly describe the problem, *starting from the beginning.*

❑ **What is the CAUSE of the problem?**

For example, your immediate problem may be that you need more computing time. But the *cause* of your problem is perhaps that you want to determine the best ordering of a disordered compound and that you anticipate that this will require running many calculations.

❑ **What are all the possible solutions to the problem?**

List *all* possible solutions that you can think of, including those that you may not know how to implement or think might not work. If you don't have a solution, list all the avenues you tried (e.g., Google search terms) to find one. If you already tried some solutions but they failed, summarize that information here.

❑ **What solution do you suggest?**

Provide your reason for suggesting this solution.

Software help groups

If you have problems with software, and in particular the software maintained by our group and our collaborators, you should contact the appropriate help group. The documentation for the software will list what that channel is; if not, try the Github Issues page. If you contact Anubhav, make sure you address the four questions above as well as provide everything needed (files, test code, etc) to quickly reproduce and debug the problem.

Two other ways to get software help that are more self-guided are:

- If you are having trouble using a particular class or function, look for unit tests within the code, which often demonstrate how to use the class or function
- If the class or function has a unique name (e.g., MaterialsProjectCompatibility), another option is to both Google *and* search on github.com for the particular class/function. The github.com search will often reveal code snippets from users all around the world.

Face-to-face meetings

Sometimes, it is best to simply meet face-to-face rather than try to solve a problem or plan a project over e-mail. If you would like a face-to-face meeting, you should first e-mail me and tell me why you'd like to meet. If a meeting is in fact the best solution, we will work out a time and place to have the meeting. Note that if there is something really troubling you, or if the issue is of a more personal nature, please do not hesitate to request a meeting.

Note that I will stop by your office from time to time to ask if you'd like to talk about anything as well as try to schedule meetings with you from time to time just to see how things are going. Those are good times to speak up if there is anything to discuss in person or if you'd like to schedule a meeting for another time.

Friday Afternoon Tinkerings (FATs)

"You'll learn infinitely better and easier and more completely by picking a problem for yourself that you find interesting to fiddle around with, some kind of thing that you heard that you don't understand, or you want

to analyze further, or want to do some kind of trick with - that's the best way to learn something".
- Richard Feynman

"...it is certainly all right and potentially very productive just to mess around. Quick uncontrolled experiments are very productive. They are performed just to see if you can make something interesting happen".
- E.O. Wilson

Long-term members of the group (*i.e.*, graduate students and postdocs) are encouraged to spend Friday afternoons on a project of their choosing. This is similar to the "20% time" afforded by companies like Google. You can pick any project you think is important or interesting, as long as it is related to our group and somewhat related to your main project theme. It is best if the project is scientific in nature, but it can also be software related (*e.g.*, to try a new visualization library or to improve the scaling of calculations at supercomputing centers). The most important aspect is that you should be able to get a result (whether positive or negative) in a short time (see "metrics for successful FATs").

You are the boss for your Friday Afternoon Tinkerings (FATs).

FAT rules

- To initiate a Friday afternoon tinkering, simply email Anubhav to let him know that you are going to try this. This will also serve as a reminder to him to leave you alone on Friday afternoons.
- At the end of every month that you are doing a FAT, you will be expected to provide 3 slides that describe your project and its status.

- Based on the slides, Anubhav will suggest what to do next. Regardless of Anubhav's suggestions, you are allowed to continue for another month (2 months total) on the same project theme.
- At the end of 2 months, Anubhav will either (i) tell you to stop working on this particular project, (ii) ask you to continue hammering, or (iii) make your project more official and extend your time on it.
- One Friday afternoon tinkering at a time - pick the most important or most exciting one if you have several ideas.

Metrics for successful FATs

The main metric for success of a FAT is whether you were able to prototype and test an idea. It does not matter as much whether the outcome was positive or negative, so long as you were able to obtain a clear result.

For example, let's say your project is to represent crystal structures as graphs. Over 4 afternoons, you do basic research and develop some rudimentary code to represent crystals as graphs. You include these graphs as descriptors for predicting a several materials properties, discover the results are not so good compared to existing descriptors, and conclude that the idea probably doesn't work very well after all. This is a ***successful*** project, despite the negative outcome, because you performed a real experiment and got a result.

As a counterexample, let's say you are interested in developing a predictive theory for metastable states. You spend the first 4 afternoons

doing literature research and talking to colleagues about how to proceed, spending most of your time brainstorming. You spend 4 more afternoons and you think you might have sketched out a good plan of how to tackle this problem. This is an ***unsuccessful*** project because you did not actually build anything or test any ideas. Even if you felt this was productive research, this was not a FAT project.

Main message: you must prototype, test, and gather data during your FATs!

Our computing systems

Our group's main computing resources are:

- NERSC (the LBNL supercomputing center, one of the biggest in the world)
- Lawrencium (starting sometime in 2017, our group will own 4 high-performance dedicated nodes on this cluster)
- Argonne Leadership Computing Facility (sometimes)
- Oak Ridge Leadership Computing Facility (sometimes)

At any time, if you feel you are computing-limited, please contact Anubhav so he can work with you on finding solutions.

NERSC

To get started with calculations at NERSC:

1. Ask Anubhav about whether you will be running at NERSC and, if so, under what account / repository to charge.
2. Request a NERSC account through the NERSC homepage (Google "NERSC account request").

3. Someone at NERSC will validate your account and assign you computing hours
4. At this point, you should be able to log in, check CPU-hour balances, etc. through "NERSC NIM" and "My NERSC" portals
5. In order to log in and run jobs on the various machines at NERSC, review the NERSC documentation
6. In order to load and submit scripts for various codes (VASP, ABINIT, Quantum Espresso), NERSC has lots of information to help. Try Google, e.g. "NERSC VASP".
    a. Note that for commercial codes such as VASP, there is an online form that allows you to enter your VASP license, which NERSC will confirm and then allow you access to.

Lawrencium

Lawrencium is somewhat different than NERSC in that we must maintain our own software environment and pre-installed binaries for common codes are not available. Thus, maintaining the software environment at Lawrencium is a group endeavour. Our negotiation to purchase nodes on Lawrencium is currently in progress. This handbook will be updated when we have completed the purchase and it is ready for the group's use. Note that if our purchased nodes is not enough to sustain our computing needs, it is also possible to pay per CPU-hour on Lawrencium as well as to increase our purchase order. Ask Anubhav if you think you need this.

ALCF and OLCF

Both ALCF and OLCF are "leadership computing facilities" meaning that they operate some of the fastest computers in the world. The strength of these facilities is that they offer very large amounts of computer time available for users; the weakness is that is much more difficult to use these computers. Therefore, it is generally only worth using these resources if you have a significant amount of computing to do (*i.e.,* at least 1 million CPU-hours). Contact Anubhav if you think an account on ALCF or OLCF would be useful.

Resources for learning new topics

Slack

If you have a specific question, sometimes the easiest solution is to post it to the Slack group and crowdsource the answer.

Books: LBNL, UC Berkeley, and public libraries

As an LBNL employee, you can get access to almost any book you'd like using various channels:

- LBNL has its own library, but it is small and unlikely to contain the book you want.
- LBNL employees can borrow books from the UC Berkeley Library collection using your LBNL ID. You can even reserve the book online and have it delivered to the LBNL library, saving you a trip down to campus (this is what I do).
- Your local library (e.g., Berkeley Public Library) often participates in Interlibrary loans. For example, the "Link+"

system at Berkeley Public Library connects to many other university libraries in the area. Again, you can have the items delivered to your local library. This service is extremely useful when an item cannot be found at UC Berkeley or if that item has a long waiting list.

You can also purchase books with research funds.

Materials Science

"Don't despair of standard dull textbooks. Just close the book once in awhile and think what they just said in your own terms as a revelation of the spirit and wonder of nature".
- Richard Feynman

It can be difficult to find resources that explain concepts in materials science clearly. Often, struggling through multiple attempts to understand a topic using several different resources in a patchwork and non-linear fashion is the only way forward. That said, the resources listed below are particularly helpful.

Density functional theory

For beginners to density functional theory, I would recommend the book "***Density Functional Theory: A Practical Introduction***", which truly achieves what it states by providing physical insights and relevant information rather than just list equations. A copy is available within the group.

If you are interested to explore applications of density functional theory, you might try the E-book from Professor John Kitchin:

https://github.com/jkitchin/dft-book
Note that this book has chosen to use the Atomic Simulation Environment (ASE) to set up simulations rather than the pymatgen code that we prefer, but that is a minor point.

Finally, for specific calculations with VASP, there are resources online from a 2016 workshop conducted at LBNL, including videos and training materials:
http://www.nersc.gov/users/training/events/3-day-vasp-workshop/
http://cms.mpi.univie.ac.at/wiki/index.php/NERSC_Berkeley_2016

General materials science topics

To gain a quick introduction to many topics in materials science, you might try the (horribly-named) web site from the University of Cambridge: Dissemination of IT for the Promotion of Materials Science (DoITPoMS):
https://www.doitpoms.ac.uk
The explanations in this site are very basic, but what they do cover is well-explained incorporates helpful visuals. Although you won't ever master a topic from this site, it is often a good starting point that can help you unlock a more intermediate resource.

Online tools

A nice tool for visualizing phonon modes is:
http://henriquemiranda.github.io/phononwebsite/phonon.html

Computer programming

Note that there are usually many excellent resources to choose from when learning computer science topics. You usually have the flexibility of choosing to learn from a book, a video series, or even interactive tutorials like ***www.learnpython.org***. Use the list below as potential starting points, but there exist many other high-quality alternatives you can find on your own and may be even better-suited to your needs.

Python

For beginners to Python, you might try the book "***Head First Python***". It is a fun and easy introduction to Python. For advanced programmers, you might try "***Expert Python Programming***".

Data mining and Data Analysis

For learning basic data mining libraries (*pandas*, *scikit-learn*) as well as some skills like using *git* and *Github*, you might try the online YouTube videos from Kevin Markham, an educator at Data School. These videos also do a good job of pointing you to supplementary material:
https://www.youtube.com/user/dataschool
https://github.com/justmarkham

You might also try the book "***Python for Data Science For Dummies***" (please note: this is different than "*Data Science for Dummies*").

Finally, you can try working your way through the *Machine Learning In Materials tutorial* in the Appendix of this handbook.

MongoDb

A (now somewhat old, but still clear) resource for beginning to use MongoDb is the "*The Little MongoDB Book*":
https://github.com/karlseguin/the-little-mongodb-book

There is also an extensive library of webinars on MongoDb on their official web site.

Seven questions for self-assessment

At LBNL, there are no regular performance reviews required for interns, graduate students, or postdocs. However, you might be curious as to whether you are on the right track from a professional standpoint. You can ask Anubhav to give you feedback periodically, and you should do this at least every 6 months or so. However, here is a cheat sheet of seven things he considers when thinking about your progress.

1. How self-driven is your work?
    a. Almost all of what I do was sketched out by my advisor; my job is to implement those ideas
    b. I originate maybe 50% of the ideas that I work on; the other 50% are from my supervisor
    c. I am far ahead of my supervisor in understanding and guiding my project, so it's necessary that I conceive/design/imagine/build most of what I do
2. When am assigned a task, I usually complete it:
    a. To minimally achieve the original goal, thus often requiring future revision; OR very late; OR usually by getting someone else to solve most of the hard parts for me

    b. approximately on time and well-tested and robust so that I know that my solution works under diverse situations. I can declare "mission accomplished successfully" the vast majority of the time.
    c. To an even higher quality standard than asked for and/or much quicker than expected
3. Compared to others in the group, I:
    a. help them less than they help me
    b. help them about the same as they help me
    c. help them more than they help me
4. Regarding independent Friday Afternoon Tinkering projects, I have completed:
    a. None
    b. About one every 6 months
    c. At least one every 3 months
5. I have submitted to a journal:
    a. No papers in the last 9 months
    b. One pretty good paper in the last 9 months
    c. Multiple papers, or one stellar paper, in the last 9 months
6. Will my main work serve as a lasting contribution that others will use and refer to in 5-10 years time?
    a. Honestly, probably not
    b. Probably 5 years, 10 years is a stretch
    c. There is a good chance my work will remain important even after 10 years
7. How is your passion and enthusiasm level?
    a. I feel burnt out or demotivated
    b. About normal

c. I feel extremely excited and happy about work

If your answers are mainly (a), the questionnaire is probably telling you something that you already know -that you should take some time to reflect on your situation. You might also schedule a meeting with Anubhav to discuss things. If you are answering mainly (b), then you are likely doing fine but it may be worth brainstorming if it's possible to move into category (c) for one or more of your responses (although it's certainly not expected that anyone get a "perfect score" on this assessment). Otherwise, continue the great work!

Fun things to do in the area

It would be foolish to spend your time in the Bay Area without exploring some of its recreational activities. Although there are probably hundreds of online and print resources that can help guide you to things to do, here are a few select ones to start you off:

- ❑ Berkeley Marina (walking) - either the boardwalk or the Cesar Chavez loop
- ❑ Ohlone Parkway Trail (easy bike)
- ❑ Bike the Golden Gate bridge to Marin (longer bike)
- ❑ Indian Rock park
- ❑ Detour App - guided tours for locals through your phone
- ❑ Berkeley Jazz / Theater
- ❑ UC 50% off performing arts at Zellerbach Hall
- ❑ SF Film Fest
- ❑ Baker beach walk up to Golden Gate Bridge
- ❑ Ice Cream - Mitchell's, Humphrey Slocombe, Bi-rite, Ice Cream Bar (skip the line, go directly to the back bar and order a "New Orleans Hangover" - non-alcoholic)

- ❑ Muir woods
- ❑ Drive up to Mount Diablo
- ❑ Hike - Stinson Beach / Matt Davis trail
- ❑ Muir Beach Lookout
- ❑ Wine country / Sonoma
- ❑ Point Reyes Lighthouse - Elephant Seal season Dec - Feb
- ❑ Route 1, Big Sur, 18-mile drive. Would very much suggest going down to Bixby bridge area at least once.
- ❑ Explore Monterey and Carmel-by-the-Sea
- ❑ Lake Tahoe - skiing in the winter, hiking/biking/cruises/tourism/casinos in summer

Appendix A: Finding a place to live

Note: It is encouraged that readers of this document also contribute to it when they have gained experience with their own housing situation by adding comments or emailing Anubhav with their suggestions.

Resources for finding housing

Unless you are part of a program that assists you with finding housing, you must find a place to live on your own. Some resources for finding housing include:

- ***http://classifieds.lblops.wpengine.com/?classifieds_categories=rentals-and-roommates***
- ***http://www.zillow.com/***
- ***https://calrentals.housing.berkeley.edu/***
- ***http://sfbay.craigslist.org/search/eby/apa?***
- ***http://csee.lbl.gov/Housing/Other_Housing_Resources.html***

You can join the LBNL postdoc mailing list (***https://calmail.berkeley.edu/manage/list/listinfo/postdocnet@lists.berkeley.edu***). You do not have to be a postdoc to join. Keep an eye on the posts for room/apartment to rent as well as moving sales.

Notes on the Bay Area housing situation

The Bay Area is a very nice place to live, which has the consequence of many people wanting housing here. Thus, one of the few problems with this area is the very high price and competition for housing. Some things you should be aware of:

- prices in the $2000/month range for a very basic apartment are normal - and can easily go up from there.
- buildings tend to be older, and amenities like dishwashers and heating/cooling are hard to find.
- it is normal to have a lot of competition for a place such that you must agree to a lease on the spot or risk losing out. Examples:
    - Anubhav thought he had finalized a place to live for his first year in the North Berkeley area, but during the signing period another bidder put in an offer for $300/month greater and he thus lost the place.
    - One of Anubhav's postdocs thought he had finalized a deal for a place to rent but was late to an appointment to meet with the owner and, even though he texted about the situation somewhat in advance, ended up losing the offer on the spot for this single mistake.

You might not expect these kinds of situations unless you are from a similar area like NYC, so please be aware of them.

Commuting

Note that if you use public transportation daily, you should consider signing up for LBL's program which lets you deduct a bus or BART pass as a pre-tax expense. See ***http://www.wageworks.com/*** for more info.

Biking here is common and there are many bike lanes and shared car/bike routes, but you still need to be careful as biking to the lab will mean going through traffic. The LBNL shuttle has bike racks so you can bring your bike up to the lab with you on the shuttle rather than bike uphill.

Note that the Nextbus app and website will give times that the LBL shuttle (and also city buses) are anticipated to arrive at various stops.

If you are in a rush or just need to get around town, Uber and Lyft are apps that can help get your a ride; the fees tend to be pretty low, especially with UberPool if you're not in a hurry.

General suggestions when evaluating a place to live

- Look for the nearest grocery store
- Look for the nearest pharmacy
- Do a search for restaurants. Often, the density of restaurants in a place will tell you whether there are other things there as well.

- Perhaps do a Google Street View walk-through of the neighborhood
- Do a Google Transit search on how to get to the lab. Note that to get to the lab itself, you cannot take public transportation. Instead, there is a lab shuttle from several spots in downtown Berkeley and near campus, so you might want to gauge how to get to the nearest shuttle stop. Google "LBL shuttle map" to see the locations of the stops.
- Remember that Uber is very convenient in the Berkeley area, so not everything needs to be ideal location-wise if you need to just get somewhere once in awhile.

A note about UC Village

Many postdocs, especially those with families, find that UC Village (sponsored housing from UC Berkeley and LBNL) is a nice place to live and also enjoy the community. Anubhav doesn't have any personal experience with UC Village so it is best to research for yourself through a Google search.

What are the different neighborhoods like?

Our group maintains a document that is separate from this handbook about what different neighborhoods are like. Please ask Anubhav for it, and don't forget to ask follow-up questions on Slack!

Good luck!

Appendix B: Purchasing a computer

Most long-term appointments (graduate student, postdoc, staff) will mean purchasing a new computer. **Short-term appointments (e.g., internships) will not involve a computer purchase unless otherwise stated - you will instead receive an excellent computer from the group's stock.**

Mac, Windows, or Linux?

You should buy a Mac, and probably a Macbook. Although this sounds extreme, and may even induce strong feelings if you are used to a different system, in practice this has never been as much of a problem. Note that I am not an Apple fanatic but simply find that these are the best systems for our type of work because they contain many of the advantages of both Linux and Windows systems in a single package.

Why not Windows? I used Windows for a very long time; it is nice, but a couple of things make it non-optimal for our work. There is no native Terminal, which you will use heavily, and programs like Cygwin are poor substitutes. Certain seemingly minor decisions made by Windows (directory slashes, line endings) are different than those from Linux, making interoperability between Linux/Mac and Windows systems more problematic (e.g., copying files to and from supercomputing centers requires auto-converting line ending format).

Why not Linux? Linux is fine, but Microsoft Office is not available (which is used by us and most of the materials science research world)

and OpenOffice is a poor substitute. Certain videoconferencing software doesn't work well with Linux.

How about Mac? I have my complaints about it, as they are catering more to the general consumer and less to developers. Thus, you really need to spend some time setting up your Mac to make it productive for power users. But for the moment it remains a very good compromise between Linux-like and Windows-like and thus forms the basis for our workstations.

Preliminaries

Here is how to purchase a computer at the lab. Before we begin, a few notes:

- In terms of the mechanics of purchasing:
    - use LBNL Ebuy (not Ebay) wherever possible - you need to be on the lab network (onsite via an ethernet cable) or be connected via the VPN
    - use Amazon, etc. to buy various components if not available via EBuy
- The laptop is government property; you are expected to return it to the group when you are done working at LBNL. Note that Mac computers make it very simple to transfer everything over to your next computer.
- You are free to take your laptop home, on trips, etc., unless you are an intern in which case other restrictions may apply from the internship program.
- The lab receives your computer and tags it before sending it over to you.

- You **must** back up your computer very regularly (at least once per week). This is simple using the Time Machine app. There are zero excuses for not doing this.

Selecting a computer, monitor, and accessories

Your computer workstation is one area where you should just get whatever you think will make you most productive and not care about cost. Seriously, just get what is best and do not worry about cost.

For the computer, you should select a Macbook Pro (any screen size) as mentioned above. You can use the Apple website to browse details. I use a 13" Macbook Pro. It is powerful enough to do serious work and light/small enough to use on a plane. A 15" Macbook Pro is also a good choice. If you would like to get anything other than a Macbook Pro, talk to Anubhav.

For the monitor, I use a single Thunderbolt display but this is no longer available. Thus, just find some other high-quality, top-notch monitor. Note that one big screen is usually better ergonomically than dual monitors, and you can use the "Spaces" feature of Mac to quickly flip between virtual screens if really needed.

For accessories, make sure to get appropriate dongles:

- A VGA adapter dongle
- An ethernet cable adapter dongle
- A presentation tool, *e.g.,* Logitech R800
- A Time Machine hard disk (for backup), I have previously used the Western Digital "My Book for Mac" that is 2-4TB in size.

- A keyboard. I suggest Apple Wireless Keyboard since I like the feel of Mac keys and I also like a consistent feel between my laptop keyboard and my desk keyboard. If you prefer a larger or ergonomic keyboard, you can get that.
- A mouse/trackpad. I suggest Apple Magic Trackpad. Note that I've found that a mouse is better on Windows but a trackpad is better on Mac. The reason is because the Mac OS has really customized a lot of the interface for the trackpad (e.g., gestures). I also value consistency between my laptop and desk workstation. After awhile you get used to doing everything on your trackpad even if you were previously very productive/accurate with a mouse on Windows.

Making the purchase

1) Provide all the details of your selections in an email and send to Anubhav. If all looks OK, he will give you a project and activity ID.
2) Go to eBuy, and for items available there, add them to your cart and submit the requisition with the project and activity ID, and SAS approver as Micah Liedeker.
3) For items not available on eBuy, contact esdradmin@lbl.gov (and cc Anubhav) to obtain a procurement form. Fill it out with item details (Vendor, website, price, etc.) and send it back to her.
4) If you select the overnight shipping option (ask Anubhav about this and the related extra costs) most parts, except the computer, will arrive within a week to 10 days. The computer needs to be tagged by the lab, so with overnight shipping, it

should arrive within 2 weeks. Ideally, you will select your computer well before arriving at the lab and won't need overnight shipping.

Appendix C: Setting up a new Macbook

Installing Python development environment

The best way to manage Python installations these days is a "conda env". This will allow you to manage different Python "environments", where each environment is a set of libraries that you have installed. For example, you can have one environment that uses Python 2.7 and has certain library versions installed, and another environment that uses Python 3.5 and has other libraries installed. Another advantage of conda environments is that you can apply the same procedure on NERSC and other computing centers that support conda.

How to do this:

- Follow the online instructions on installing a conda environment and see modifications below:
    - ***http://conda.pydata.org/docs/using/index.html***
    - (probably) prefer to install the "miniconda" version rather than anaconda
    - (probably) prefer to install "miniconda 3" rather than "miniconda 2". Both will work fine and allow you to do everything the other one does so don't stress too much about this decision.

- (probably) When creating environments, create at least one python 2 environment using the "python=2" parameter. It is up to you whether you want to work in Python 2.x or Python 3.x. For the moment, Anubhav prefers 2.x backward-compatible code for most base libraries (e.g. FireWorks), so if you use 3.x as your main environment, make sure your syntax doesn't depend on the newer features. See next bullet point for more.
- When creating environments, use a command like this (note that this also installs recommended libraries):

```
conda create --name py2 python=2 numpy
matplotlib pandas flask pymongo scipy
scikit-learn jupyter plotly
```

- If you want a reference guide to conda commands, try: ***http://conda.pydata.org/docs/using/cheatsheet.html***

Install high-throughput computation environment

Our group has a set of base codebases used for performing high-throughput calculations. Note that if your project does not involve high-throughput calculation, you may need only one or two of these libraries installed – contact Anubhav if you are unsure.

- Install the following packages using a combination of `git clone >>REPO_NAME<<` and `python setup.py develop`. Start with:

        - `git clone https://www.github.com/materialsproject/fireworks`
            - You might need to generate an ssh key for the git clone command to work:
                - `ssh-keygen -t rsa -b 4096`
                - no password is probably OK unless you are security conscious
                - add your SSH key to your Github profile
        - Then: `cd fireworks; python setup.py develop`
        - Repeat the process above but replace "fireworks" with:
            - pymatgen
            - pymatgen-db
            - custodian
            - atomate (note: this is on the hackingmaterials github site)
            - matminer (note: this is on the hackingmaterials github site)
- If you want, you can automatically source activate your environment in your .bash_profile file. This will automatically load your environment when you open a Terminal. Otherwise, you will start off in your default Mac Python and will likely cause you a lot of confusion

Configure Pycharm IDE

An IDE allows you to be a much more productive coder. It is like a text editor but contains many useful keyboard shortcuts, code-completion

tools, refactoring tools, and debugging/profiling tools to help you be more productive.

- Download Pycharm professional
- Get an activation license from Anubhav
- Configuring PyCharm - unfortunately no written instructions in this version of the Handbook.

Note that there are some advanced programmers that know their way around an IDE but still prefer an editor like vi or emacs with appropriate plugins. This is fine so long as you have first tried an IDE for a few months and really tried to make use of it. It is not fine if you are simply comfortable with other tools but never seriously tried using an IDE.

Other things to do

- Set up your Time Machine backup (make sure you have purchased or received an external hard disk).
    - ***https://support.apple.com/en-us/HT204412***
- You can also set up an online backup plan (e.g., Crashplan or Backblaze) to provide you with a second backup.
- Install MongoDB.
- Purchase Microsoft office from LBNL software distribution. Anubhav currently prefers Office 2011 due to stability and usability issues in the new subscription version.

Appendix D: Some notes on using a Mac from Anubhav

Basic setup

- Macbook Pro 13" laptop
- Thunderbolt Display (now discontinued)
- Apple keyboard
- Apple Trackpad - less precise than mouse, but can be very productive if you learn all the gestures (e.g., for web browsing back/forward, for mission control, for swiping between different Mac "Spaces")

I use an Apple keyboard and Trackpad so that typing/navigating is similar whether I am at my workstation or whether I am on my laptop.

Early on, I turned up my Trackpad speed all the way to the max. This means I can very quickly move the cursor all the way across the screen. It took a few days to get used to this very sensitive setting but now I don't even notice it (when other people use my trackpad, they usually freak out…)

There are many options I set to make OS/X more oriented for power users. For example, my Finder window shows directory paths at the bottom, I have sidebar shortcuts many important locations, I display hidden files, I have a shortcut to copy the path of the current Finder location to the clipboard, etc. There are many settings like these for

various built-in OS/X apps, but unfortunately I don't remember them all. Getting a good Finder setup is probably the most important.

Apps I use for programming

- I use the PyCharm IDE. Things I like about PyCharm include:
    - underlining errors
    - underlining code "lint", e.g., spacings that do not follow PEP
    - code highlighting / editor features (e.g., when you open a CSS file, lines of code that define a color automatically display a swatch preview of that color)
    - a nice and powerful search tool (regexes, find/replace in certain files, easily filter through results visually and categorize by what type of file they occur in)
    - autocomplete (ctrl+space)
    - autofix errors, i.e. red underline stuff (option+enter)
    - follow definitions of variables, methods, classes (Cmd+b)
    - quickly open classes (Cmd+o) and files (Cmd+shift+o) and variables (Cmd+option+o)
    - go back to previous/next file being edited like forward/back on a web browser (Cmd+[or Cmd+])
    - the "find usages" command
    - code refactoring
    - structure view of code. I usually have "Project" view at left of window, code in middle of window, "Structure" view at right of window, and "Todo", "Terminal", and

"Python console" at bottom of window (along with search results).
    - debugger (sometimes)
    - easy IPython console to test code snippets
    - there are other commands that I use, but those are the ones I use most often
- MongoHub (for visually exploring Mongo databases)
- Gitbox (I almost never use the Git command line; Gitbox is unique in that it is really easy to preview changes to the remote before pulling them in. It is also the most intuitive Git tool I know of)
- Patterns (for tricky regexes)
- Cocoa JSON Editor (for examining large JSON)
- Balsamiq Mockups - wireframes

Apps I use for Science

- CrystalMaker (and sometimes Vesta) - crystal structure visualization
- Mendeley - reference management
- MS Office Suite

Apps I use for working more quickly

- Alfred - application launcher, quick file opening, quickly go to a web site. Note that if you don't use Alfred, the built-in Mac Spotlight now includes some of its features.
- Trickster - for easily calling up recent files, e.g. drag a recent file from Trickster into an email

- Default Folder X - the most useful feature of this is that it can add a sidebar to your save dialog that lets you access recent folders. This is 95% of the time where I want to save something.
- Fantastical - for quickly scheduling meetings or looking at my schedule

Apps I use to keep things organized

- Evernote
- 2Do - allows for complex todo lists, but also easy to use and intuitive. All my tasks are managed here.
- Screenshot Plus - Mac widget for quickly capturing screenshots (if like me you can't remember the keyboard shortcuts)

Misc Apps I use

- Bartender - allows you to clean up and reorganize your (top) menu bar; especially useful on the small 13" screen
- ShiftIt - keyboard shortcuts for half-screen, full-screen, etc. like Windows has had since Win7
- Mousepose and IMovie - screencasts
- Tomato One - if I find it hard to be productive or am avoiding doing something, I revert to Pomodoro method sometimes
- Focus - for sometimes restricting internet browsing if I really can't focus (usually combined with Tomato One)
- Safari for web browsing (I find the experience to be very visually smooth and pleasing, e.g., when paired with Trackpad Gestures)
- Pocket - for saving web pages to read later, and then usually never getting around to it

- Time Machine - not only for backups, but also for sometimes recovering past versions of files that might have gotten accidentally changed / overwritten.
- CrashPlan - online backup (also consider BackBlaze)
- Inbox When Ready - a Chrome extension that helps control the flow of your email (requires checking your GMail via Chrome)
- Spotify - music
- Pixelmator - image editing

Appendix E: Our open source software philosophy

"If you want to go fast, go alone. If you want to go far, go together".
- Attributed to an African proverb

Although we develop both open and closed source pieces of code in our group, we try our best to release any software that is potentially useful to more than one personas open source. This ends up being almost all the software that we write except perhaps code written to conduct a specific scientific analysis.

Benefits of open-source software include:

- authors can include the code in their portfolio for future job applications
- you get recognition from the community of users of your code as well as personal pride
- more users means more bug reports - this sounds scary but is in fact very useful and important for your own research

- outside developers can contribute fixes and features, so your code gets better for free
- much less friction - easy to share code, fork it, etc. without needing to set up permissions or access. Easy to distribute and install the code, e.g. via PyPI
- many services like CircleCI and PyCharm offer their products for free when the codebase is open source. Not only does this save money, it more importantly saves a lot of time in coordinating purchasing requests that need to be renewed.
- your own programming will automatically improve because your code is open source and public. You will be more likely to write documentation and write clean code if you know it is for the world and not only for yourself. This will also encourage writing the code in a more general manner rather than specific to your application.
- you can write a paper about your code whenever ready. There is no separate process of "making the code open source" if it is already open source from day 1.
- it is the right thing to do for the betterment of the research community!

Clarifying common misconceptions about open source code:

- Writing open source code almost never exposes you to getting scooped or having some outsider leapfrog you in research. First of all, it is very rare that an outsider will use your code rather than make their own, especially if you do not advertise your code. Most of the time, you will have the opposite problem - i.e., to convince people to use and trust your code. Second, as the code author you are the expert in the code. Even when there

is an outside user, it is rare that they are as proficient as you in the use of the code. Third, the majority of people are friendly and not as manipulative as you may think.

- Open source code doesn't need to be perfect, nor does it even need to be any good. Often people think that they will make a code open source when it is "ready". This is not the right approach; code does not need to be "ready" to be open source.
- Publishing a code as open source doesn't mean that you need to support the code or vouch for its correctness. You are offering the code publicly without any guarantees whatsoever, and you don't have any additional obligations to anyone. However, if you actively want your code to be used by the community and extended, then be prepared to document and support your code, and to help users and resolve their problems. But this is a separate decision. It is perfectly OK to have an open-source code for which you provide no support so long as you don't try to advertise it for more than it is.

Appendix F: 10 ways to write better code

There are many, many books and articles on writing better Python code. Please use those if you want to really desire to become a good programmer. Here, I am just focusing on some of the most basic things that I think are particularly relevant to the types of scientific programmers we get in the HackingMaterials group.

Note: I used this site: ***http://markup.su/highlighter/*** to help write code blocks with coloring. For additional flair, you might also try using: ***http://instaco.de***

1. Prefer data structures that don't require memorizing array indexes.

Don't use a data structure (like a list/array) that requires one to remember that "index 8" is the species string and "index 1" is the coordination number.

Bad:

```
my_data = ["Fe2O3", 6, 5, 43, 4.1]
cell_volume = my_data[1] * my_data[2] * my_data[3]
is_insulator = my_data[4] > 3
```

Better:

```
my_data = {"formula": "Fe2O3", "a": 6, "b": 5, "c": 43, "band_gap": 4.1}
cell_volume = my_data["a"] * my_data["b"] * my_data["c"]
is_insulator = my_data["band_gap"] > 3
```

Notice how much easier it is to follow the logic of the code in the second example?

You can also use a pandas *DataFrame* object if you have lots of data and don't want to repeat the same column headers many times.

2. Document all classes and methods in a standard format

It is really important that all classes and methods are documented. Code is much more often read than written (a tenet of Guido van Rossum), so it needs to be readable and understandable. If you don't know what format to use, try the below:

http://sphinxcontrib-napoleon.readthedocs.org/en/latest/example_google.html

You should also pay attention to the format already being used by a particular package.

3. Inside of classes/methods, write code that is readable without documentation whenever possible

This is usually achieved by writing descriptive variable names, function names, and good interfaces to functions. As a small example, why do this (requires documentation to tell user what my_d represents):

```
my_d = {"Mg": 3, "Ag": 8, "Li":4}  # dict of el. symbol to coord. number
all_element_symbols = my_d.keys()
all_coordination_numbers = my_d.values()
```

when you can do this (same clarity in first line, better clarity in last two lines, no documentation):

```
elsymbol_coordnum = {"Mg": 3, "Ag": 8, "Li":4}
all_element_symbols = elsymbol_coordnum.keys()
all_coordination_numbers = elsymbol_coordnum.values()
```

Of course, sometimes you will need to write documentation!

4. Follow PEP formatting guidelines

Following proper code formatting helps clarify your code. There are a billion PEP rules and you don't have to follow all of them. But at least get the basic ones correct. Like:

- functions/methods are named like this: `my_very_first_method()`
- classes are named by CamelCase like this: `MyVeryFirstClass`
- python files are named like this: `my_very_first_file.py`
- python modules are named like this: `my_very_first_module`

If you use an IDE like PyCharm, it will detect, underline, and automatically fix most of the worst cases for you, so learn to use the feature. There are also tools like PyLint that you can use separately from IDEs (PyCharm basically has a nice wrapper around PyLint).

Also, don't use ugly code separator comments like "`##########################`" or ASCII art - stay clean and professional.

5. Use standard file formats

Use JSON or YAML most of the time if you need a file format, *e.g.,* for a settings file. XML is very heavyweight and quickly being outdated. Don't invent your own strange conventions (like CIF or any other custom file format).

6. Wrap exe code in 'if __name__ == "__main__":'

Python often runs your file even when you don't intend it to, e.g. when loading a module or importing some component of your file. It is

important that you don't run code as a "side-effect" of this. Use the `if __name__ == "__main__"` wrapper to prevent this.

7. Be aware of Python gotchas, in particular mutable default arguments

Do you see anything wrong with this?

```
def append_to(element, to=[]):
    to.append(element)
    return to
```

If you don't see it, then you're going to get hit with some strange and difficult to pinpoint bugs downstream in your code.

This is a common Python gotcha (there is lots of discussion online about it)
http://docs.python-guide.org/en/latest/writing/gotchas/
https://pythonconquerstheuniverse.wordpress.com/category/python-gotchas/

8. Write unit tests

Scientific researchers often don't write tests because (i) they don't write large, complex code with many moving parts or many different authors, (ii) they are overconfident about their ability to write correct code, (iii) they feel this will slow them down. Professionals write unit tests because they know that the longer and more complex a codebase becomes, and the more users it has, the more likely that something is going to go wrong down the line and the greater the dividends that are paid from writing unit tests. Unit tests allow code to be automatically tested for bugs every single time anyone makes a commit (continuous integration)

and has demonstrated its value many times over in the large production codes that we use and develop - even (and perhaps especially) for ones required to do complex tasks on a deadline.

9. Throw exceptions rather than returning coded results

One of the most common beginner mistakes is to think that their code should never throw Exceptions or Errors. Perhaps this is because in the beginner's mindset, Exceptions are associated with bugs (e.g., they run a code with a bug and see an Exception, so Exceptions are bad). Another issue is that beginners never want their code to interrupt the operation of whomever is running it. So rather than throwing an Exception when their code is given bad inputs, they will return None, -1, or False, so that they don't interrupt whomever is calling their code.

This is bad. If the user gives bad or nonsensical input to a function, an exception needs to be raised and the program needs to stop immediately if the user is not explicitly catching the exception. For example, if you try to use the Python math library to compute the log of a negative number [`>> math.log(-1)`], it doesn't return None or some nonsense like False or -1. It throws an Error! As a user, the error is much more useful than any other course of option. Think of the alternatives for math.log(-1):

- If the function returned -1, you would have returned an incorrect result (extremely bad). For example if your function computed math.log(x) * 3, and you gave a negative x, your function would return -3 - which looks perfectly reasonable but is completely wrong! This is the worst possible thing you can do.

- If you return None or False to avoid inconveniencing the user, you have just made two mistakes. First, the user doesn't really know that their input was bad; perhaps it is simply the math.log() function has a bug leading to the strange output. The second and more important issue is that a user might want to run the math.log() function over an array of 1 million integers, and then do a lot of complex processing after that. If math.log() didn't immediately throw an error when encountering a negative number in the 1 million integer array, then the code would keep proceeding with nonsensical results and the user might finish 5 or 6 additional processing steps downstream before the code finally chokes and dies because there are strange "Nones" or "Falses" where there should have been numbers.There are even more dangerous situations that can occur, like a second library to compute standard deviations that ignores None values in the array. Then the user has unwittingly taken the standard deviation of only a subset of the data and never even knows that there was a problem in the pipeline. At that point, it becomes extremely tedious to trace back the source of the error.

Code should fail immediately when there is invalid input. In general, the further the "distance" from the actual place where the problem originated and the point of failure/exception in the program, the more difficult and maddening the debug task. You are doing users a favor by moving program failure right to the place of the problem.

10. Prefer python lists to numpy where practical

Numpy is great, but it is often overused (leading to worse code). Numpy is great for algorithmic work, for very complex slicing of multidimensional arrays, and for a host of other things, but it is *not as good for creating basic data structures*. Here are some advantages that Python lists have:

- Python lists have cleaner built-in functions and code. There are lot of tools for Python lists, like index slicing and iterations, or functions like sum() and all() that make them very powerful while still very clean. Numpy has even more useful functions and operations than that (e.g., a built-in mean()), and sometimes you might need numpy in order to leverage those features, but there is no need to transform to numpy arrays to (for example) take the sum of an array. Master regular Python lists first before reaching for numpy because you will have much cleaner code.
- Python lists can be easily appended and modified without lots of "filler" like figuring out how long the array needs to be in advance and populating with zeros before modifying values. This again leads to much cleaner code and is much easier to write and to read.
- Python lists can be easily serialized and deserialized, e.g. to JSON format where they are native.
- Despite the claim that numpy is fast, numpy lists, arrays, etc can actually take a lot of time to initialize - maybe 100X more than default Python. Of course, if you are then going to heavy processing on that matrix, like diagonalizing a large matrix or doing large matrix multiplications, numpy will absolutely improve your overall performance, perhaps to large degree. But for simply creating a data structure or taking the sum of a list,

you will perform much worse with numpy while writing less readable code.

- Python lists are more universal; they don't require dependencies and they are readable by many more programmers.

Note that this doesn't mean to stop using numpy. Numpy can certainly do lots of things that regular Python cannot and it is an extremely powerful and useful library. But for routine file parsing (where being able to append easily is important), data representation (where serialization is important), overall code clarity (always important), and even speed for routine tasks (usually important) the native Python lists often have the advantage. So if Python lists are a chef's knife, and numpy is a swiss army knife, I am just saying that if you need to chop some onions stop using your swiss army knife. It does not make you clever to be able to do that. Learn to use the chef's knife until you actually need to open a can or do some other complex operation.

Appendix G: Hands-on exercises for machine learning in materials

There are many excellent tutorials for learning machine learning in general with Python, and some of them were mentioned earlier in this handbook. Those might be a good place to start. However, if you want to dive into machine learning for materials science or prefer a more hands-on approach, you might try following some of the steps below.

Step 1 - git and Citrine tutorial

Skills gained: git, Github, Python, MP Rest API, scikit-learn

Use an IDE (e.g. PyCharm) and invest in getting it running and set up on your system. Force yourself to learn the IDE and its features over time.

- Create a new repository in your Github account (public is fine).
- Complete Parts 1 and 2 of Citrine Informatics's blog on Machine Learning for the Materials scientist.
- Push the code to your repository. Make sure to commit to git throughout at short intervals, i.e. at the completion of every step, i.e. at least 6 commits for the tutorial (more is fine).

Step 2 - pandas and data exploration

Skills gained: pandas, plotting, data exploration

Note that the steps below should be ***easy***, *i.e.*, built-in functions in pandas for the most part that can be done in 1-2 lines of code. If you find yourself trying to write long and complicated code, you are probably not doing it correctly.

- When you are reading the data from the CSV file, read it into a pandas dataframe object.
- Use the data stored in the pandas dataframe to get summary statistics on the band gap data. min, max, mean, quartiles, etc. (look for the built in pandas function to get summary statistics)
- Make a histogram plot of the band gap data distribution.

- Add to your data frame - make a new column that is equal to the square of the band gap.
- Make a quick scatter plot of gap vs gap^2.
- Use the scatter_matrix() function to see the relationships between all quantities

Step 3 - further explorations with pandas

Skills gained: putting data into a pandas dataframe

- Rewrite the Citrine tutorial in Step 1 above (i.e. scikit learn fitting, adding features to the data, etc.) using pandas as the data structure. e.g., when you add features, it should be a new column in the data frame. What this means is that the "materials, bandgaps, and naive_features" lists should be *deleted* and unnecessary, and all 3 of these variables replaced by the pandas data frame.

Step 4 - playing with different models

Skills gained: bringing all the skills together to do a new analysis

- Get the formation energy in addition to the band gap for each compound using MPRester and put it in the data frame. So now you have columns for gap and formation energy (in addition to the one for material).
- Test if also including the formation energy in your predictor set improves your model of the band gap.
- Also repeat the above with the density of the material.

- Compare the baseline errors of the different models that use the naive and physical feature sets when using just the bandgaps, formation energies, and densities, and in different combinations with each other.
- Make a quick scatter plot to visualize the correlations, if any, between the properties and compare with the baseline errors above.

Step 5 - the interactive Jupyter notebook

Skills gained: Jupyter notebook

- Create a Jupyter notebook for your code. The final product should be a nice document with all plots in-line and that clearly show all steps.

Step 6 - matminer

Skills gained: the matminer package that we developed.

- Install matminer on your system, if not already installed
- Work through the example Jupyter notebooks for matminer

Finally, give yourself a pat on the back - and think of how you can now apply your newfound skills!

Thank you!

Thank you for contributing to this handbook!

- Saurabh Bajaj
- Alireza Faghaninia
- Joey Montoya