BMD

Burton Materials Discovery
Lab

מעבדת ברטון לגילוי חומרים

Group Guide

אלף

TEL AVIV אוניברסיטת
UNIVERSITY תל אביב

Contents

1 INTRODUCTION

This group guide has two purposes, to help new members get started and to help existing members agree on the best way of working together. It is inspired by similar guides that are available on-line and many years working in different research groups all over the world.

The document is split into separate sections describing specific aspects of our professional lives at Tel Aviv University. It is arranged in the approximate order you might find the information useful. That is to say when you first arrive, Section 2: Tel Aviv will be probably of most relevance to you. Then understanding the group. Then conducting the work. Finally, creating outputs from your research.

I wrote this guide for someone with no experience working in academic research or experience of Israel, so I hope it can be useful to new arrivals at any level. It should give you an idea about the kind of expectations we have as a group and what you can expect from us in return. You definitely don't need to memorise anything in this document so don't worry. The guide will be constantly receiving updates, so please check for the most recent version. When you are finished reading it, please let me know if you have any suggested updates or changes.

The writing here is the level of English a scientist is expected to be able to understand in research so I deliberately do not try to make it easy. Please take the time to compare the English I use and any corresponding translation to improve your understanding as necessary. In this way, this document can also help establish a minimum level of English for all members.

2 TEL AVIV

Welcome to Tel Aviv! In this section I just write a brief guide to staying with us, understanding the university and finding your way around. However, the best way to find information will always be talking staff, students and me so feel free to ask :)

Tel Aviv University, (or TAU), is almost entirely contained in the main campus of Ramat Aviv.

2.1 RAMAT AVIV CAMPUS

The main TAU campus in Ramat Aviv has everything you need to have a pleasant stay in with us. We are based in the Department of Materials Science and Engineering of the Faculty of Engineering. Our offices are in the Wolfson Building in the engineering section of the main campus (see campus map). We also work quite closely with the Faculty of Exact Sciences, which houses both chemistry and physics departments. All of the departments of Tel Aviv University hold regular seminars and frequently host international visitors so, wherever your interests lie feel free to immerse yourself in the active research going on all around us.

Please also note that there are 11 exits around campus and the rest of the perimeter is fenced. All of the exits have turnstiles permitting exit all day every day but gaining entry is not always available. The so called "Ramniceanu Gate", which is labelled G4 on the campus map is usually

open 24/7 but many of the other gates are closed outside of normal working hours.

There are several convenience stores around campus depending on what you are looking to buy. Underneath the Physics and Astronomy building (X6 on the campus map) there is a stationary store that sells pens, paper, folders etc. The Anu Museum (I1 on the map) has a gift shop with some stationary too and various ornaments and interesting things to buy. Finally, if you head over to Broshim Campus you will find a small selection of stores and amenities. Broshim campus is where most of the University accomodation is located; on the ground level you will find a gym, a hairdressers and a "Victory" supermarket that has lots of groceries available. There are also a few restaurants as we will discuss in the next section.

2.1.1 CAMPUS EATING

There are quite a few canteens on campus, the one closest to us is called Yotto and is on the ground floor of the Wolfson building. This canteen is a little expensive but serves a variety of meats such as beef and chicken (all food places on campus are kosher so you won't find pork or shrimp anywhere). The cheapest canteen that I've found is called Lunchbox and is underneath the Physics and Astronomy building (X6 on the map), next door to the stationary store I mentioned previously. While the prices are typically lower, Lunchbox only serves fish and vegetarian food so you can decide where you prefer to go.

There are a few other canteens to eat but I'll just also point out that there are some nice cafes nearby for good coffee/pastries/cakes/sandwiches etc. The Anu Museum has an Aroma cafe on the ground floor. You don't need a museum ticket to enter and they have a great balcony overlooking campus which is a nice place to be on a sunny day. This place is probably the most expensive on campus however, so you may also consider visiting CafeNeto that is nestles in a little courtyard of a building between us and the main library. Either way give them both a try!

The canteens are usually open between 9-5 each day but the specific times depend on the place. However I have known them run out of food by about 3pm so don't leave it too late if you're looking for a real meal!

> **Note**
>
> If you are vegetarian, vegan, have celiac or severe allergies the canteens might not be suitable for you. Talk to me and I'll help you find what you need.

TEL AVIV UNIVERSITY
Pursuing the Unknown

Buildings & Halls

Bar-Shira Auditorium — U10
Bob Shapell School of Social Work — S1
Britannia – Cohen-Porter Family United Kingdom Building — F1
  Austrian Friends of Tel Aviv University Hall (05) — I2
  Rose and Morris Leigh Auditorium (014)
Buchmann–Mehta School of Music
Clairmont Hall — A1
  Targ Auditorium
Building for Crop Improvement
Carter – Victor and Adrea Carter Building
Chaim Rosenberg School of Jewish Studies
Check Point Building
Coller School of Management–Recanati Building — G1
  Hasan Robhi Lecture Hall (09)
  Harry Triguboff Building
  Lion Hall (104)
  Nehama Rubin Lecture Hall (105)
Dan David Building — D1
  Andrea And Martin Schlaff Lecture Hall (110)
  Anwar and Maji Shemesh Auditorium (001)
  Argentina Auditorium (003)
  Prof. Michael J. Higatsberger Hall (111)
  Sara and Felix Dumont Auditorium (002)
  Vienna Hall (112)
David Glasberg Tower for Medical Research — M1
David Azrieli School of Architecture — A2
Desenberg Wolf Building — U1
Silverstone Hall
Dolfi and Lola Ebner Auditoriums — M8
  Sigma Epsilon Delta Fraternity Auditorium (254) — I4
  Styrt Family Entrance Foyer
Mexico Building of the Arts
  Adolfo and Thelma Fastlicht Auditorium — S2
Millie Phillips Student City (see back of map)
Miriam and Adolfo Smolarz Auditorium — U2
  Ruky and Sergio Grosskopf Family Foyer
Moshe Sharett Building of Educational Sciences — E2
  Jonas and Blanche Feiner Hall (Food Court) — U3
Myers – David and Inez Myers Building for the Transgenic Modeling of Human Disease — T6
Naftali – Pever Naftali Building for Social Sciences — I4
  Paula and Rina Perlman Lecture Hall (101)
  Rudy and Erwin Guttman Lecture Hall (201)
Smolarz Family Building — T3
Sylvan Adams Sports Institute — S3
Ruth and Allen Ziegler Building for Zoological Research
Trubowicz Building of Law — M2
  Azriel Carlibach Lecture Hall (201)
  Claudia Cavezzel Birene Hall (001) — X2
  Kaplan Lecture Hall (209) — D2
  Malka Brendler Hall of Justice — U11
  S.E. Hoofien Hall (105) — U7
  Zakheim Family Hall (301)
W.A. Minkoff Building of Law — X7
Webb – Max Webb Family School of Languages Building
Wolfson Building of Computer and Software Engineering
  Claire and Emanuel G Rosenblatt Auditorium — M5
Wolfson Building of Electrical Engineering
  Haim Auditorium (101)
  Lola Litsyn Auditorium (102)
  Prof. Adu Seidman Lobby
Wolfson Building of Mechanical Engineering
  Feiner-Schonberg Student Lounge (Cafeteria)
  Philip and Zelda Tbau Auditorium — F5
  Rubinstein Lobby

Eitan Berglas School of Economics
  Malka Mozes Hall (012)
  Malka Golub-Mozes Hall (011)
Ofsir Hall (110)
Engineering and Maintenance Building
Engineering Studies Building
Eric Mitchell Student Center (see back of map)
Gilman – Aaron and Cecile Mallah Building of Humanities
  Baruch And Zeev (Bobby) Mucviman Hall (220)
  Benyamin Yerushalmi Hall (449)
Berger Hall (223)
Bernard Silver Hall (326) — F1
Drachlis Conference Hall (496)
Ruth Cheshin Lecture Hall (28)
Schotlander Hall (140)
Yona Ettinger Hall (144)

Joseph Meyerhoff Building — G1
Miles S. Nadal Home for Technological Innovation and Entrepreneurship
Lory Lokey Building
  Vicky and Joseph Safra Plaza and Entrance Hall
Isaac and Ruth Ziskind Computation Building — X1
Louis Calder Jr. Computation Center
Machinery Building – North — U5
Prof. J. Higatsberger Hall (200)
Irwin G. Beutel Entrance Hall
Nicholas and Elizabeth Slezak Auditorium — D4
Sara Racine Root Laboratory

Saul Kaplun Building of Mathematics and Space Physics — X3
Schreiber – Wladimir Schreiber Institute of Mathematical Sciences — X4
Security and Logistics Building — U8
Susan and Henry Samueli Engineering Building — E7
George S. Wise Senate Building — U9
  Raya and Josef Jaglom Auditorium
Shenkar: Chemistry – Arieh and Rivka Shenkar Building of Chemistry — X5
  Boris and Lena Melamed Auditorium
  Zöbella and Marcos Leon Holcblat Auditorium — U6
Shenkar Physics – Arieh and Rivka Shenkar Building of Physics — X6
  Abraham Lev Auditorium
Sam and Simone Mallah Student Recreation Center — M6
Sherman – Archie Sherman Building of Life Sciences — T4
  Lecture Hall in Memory of Judy Langer-Gefter (02)
Smolarz Family Building
  Sylvan Adams Sports Institute
Ruth and Allen Ziegler Building for Zoological Research

Libraries

Archeology Library — T3
Azrieli School of Architecture Library Building — A2
Bob Shapell School of Social Work Library — S1
Brender-Moss Library for Social Sciences, Management and Education — L1
David J. Light Law Library
  Cyril Light Entrance Hall — L2
Elias Sourasky Central Library
  Noah and Sarah Werbin Hall
  Albert Dov Sigal Gallery — L3
Geography Library — F6
Gitter-Smolarz Library of Life Sciences and Medicine — F8
Marc L. Ginsten Music Library — E5
Mehlmann Library
Neiman Library of Exact Sciences and Engineering — F7
Wiener Library

Points of Interest

Anu – Museum of the Jewish People — W1
Cymbalista Synagogue and Jewish Heritage Center — I1
Sylvan Adams Sports Center (see back of map) — I5
Genia Schreiber University Art Gallery — I3
The Lowy International School — A3
Mia and Mike Pinkas Accessible Learning Center — I7
Michel Kikoine Foundation Art Gallery — L3
The Steinhardt Museum of Natural History — W2
  Fabian-Cyril Boisson Auditorium — E3
Galil Plaza — I8
Rita and Chaim David Filler Garden — E1
Dan David Anthropology Garden — O38
Eva and Les Erdi Educational Gallery — O19
Yehuda Naftali Botanic Garden — E4

Outdoors

Adler Music Street — O14
Albert and Elba Cuenca Boulevard — O18
Albert and Elba Cuenca Entrance Plaza — O41
Albert Einstein Square — O27
Alexander and Antonie Moksel Promenade — O4
Alpha Omega Regency Garden — O39
Bernard Jaskarzec Memorial Garden — O23
Betty Wozniak and Sofia Blake Garden — O40
Check Point Road — O8
Juna and Bruno Mandel Square — O3
Dan Bochner Avenue — O17
David and Marlene Studer Family Garden — O5
David and Zipporah Federmann Promenade — O28
De Botton Square — O7
Dr. Marvin Schloss Memorial Garden — O1
Entin Square — O9
Esther Sidi Garden in Memory of the University's Fallen in Israel's Wars — O25
Frankel Avenue — O6
Hanna Doron Memorial Garden — O15
Henry Gildred Promenade — O11
Holocaust and Heroism Square and Avenue donated by David and Fela Shapell — I5
Jacob and Shoshana Schreiber Square — I6
Laura Schwarz-Kipp Square — I7
Levi and Fortuna Eskenazi Sculpture Garden donated by Giulia and Beniamino Matatia — L3
Lili Peyser Plaza — O30
Lowe and Marshall Garden — O32
Meir Ilan Square — O13
Troupeau de Gazelles au nom de Michel Sapon Adopte par la Famille Sapon — O29
Morris and Manja Leigh Avenue — O38
Norman, Evelyn and Irving Feintech Garden — O19
Paula and Menachem Gottesdiener Square — O31
Sam Mallah Palm Tree Garden — O3
Sarita and Noel Werthein Senate Plaza — O34
Shella and Yossi Carmel Garden — O21
Shelley and Joel Tauber Family American Honor Plaza — O36
Shlomo Rechav Garden — O22
Stanley and Helen Grosman Garden — O24
Theo and Margot Lowengart Bridge — O37
Townsend Avenue — O20
Urs and Aviva Felher Jubilee Plaza — O35
Victor and Adrea Carter Garden — O26

Gates

Austria Gate (Prof. Klausner St.) — G1
Matatia Gate (Prof. Klausner St.) — G2
Ramniceanu Gate (Dr. George S. Wise St.) — G4
Frenkel Gate (Haim Levanon St.) — G5
Josef Kryss Gate — G7
Dan and Zippi Bochner Gate (Haim Levanon St.) — G8
Josef Super Gate (Haim Levanon St.) — G9
Gate 10 (Klatzkin St.) — G10
Chella and Moise Safra Gate (Prof. Klausner St.) — G14
Noel and Sarita Werthein Gate (Dr. George S. Wise St. – West) — G16
Gate 17 (Dr. George S. Wise St. – East) — G17

Public Car Parks

P1
P2
P3
P4
P5
P6
P7
P8
P9
P10
P11
P12

Academic Units

A# Yolanda and David Katz Faculty of the Arts
E# Iby and Aladar Fleischman Faculty of Engineering
X# Raymond and Beverly Sackler Faculty of Exact Sciences
L# Lester and Sally Entin Faculty of Humanities
W# Buchmann Faculty of Law
G# George S. Wise Faculty of Life Sciences
U# Coller School of Management
S# The Sackler Faculty of Medicine
M# Gershon H. Gordon Faculty of Social Sciences
D# Multidisciplinary

L# Main Libraries
I# Points of Interest
U# University Administration
G# Gates
H# Public Car Parks
W# Outdoors
X Cafeterias
Tel-O-Fun

KEREN KAYEMET BOULEVARD — KLATZKIN STREET — EINSTEIN BOULEVARD — PROF. KLAUSNER STREET — DR. GEORGE S. WISE STREET — HAIM LEVANON STREET — CHECKPOINT ROAD — DR GEORGE S. WISE STREET — TO AVALON

2.1.2 UNIVERSITY LIBRARIES

Tel Aviv University has several libraries with communal spaces for you to sit and work or enjoy a good book! The central library is the big library does have some English language books available but they've proven quite difficult to find using the on-line catalogue. The best thing is to ask for help from a student here as they're usually familiar with the common textbooks. Alternatively, many textbooks now have on-line versions that you'll be able to access *via* the university network.

2.2 OUTSIDE CAMPUS

Ramat Aviv has it's own interesting shops, restaurants and bars to visit. One of the most useful places to know about is Einstein street. This street runs from the university in a straight line down to the beach. Between you will find many different and useful places to buy things.

Assuming you are walking from the university towards the beach, on your left behind the university dormitory (also called Einstein) there is a small supermarket which has some of the lowest prices for groceries around while still being good quality. On the opposite side of the road from here is a Super Yuda, which is a little more pricey but is probably worth checking out if you want a greater range of produce to choose from than is held by the other supermarket.

Still further down the road and on your left you will find the Ramat Aviv Shopping Mall. Here you can find all kinds of fashion brands, home ware stores, cafes and the like.

While you can live perfectly well on campus, you'd be missing out if you didn't travel occasionally into Tel Aviv. Bicycles and scooters are a great way to get around such short distances. If you are here for a

> **Note**
>
> Tel Aviv is relatively cool because of the Mediterranean breeze but the sun is still very strong! If you are easily burned be sure to keep sunscreen with you.

short time, I'd recommend signing up for one of the electric scooter rentals. They are all over the city, and very convenient to get from door to door (and are fun too!). There are a few different brands but by far the most common around the university is XXX. However, the scooters typically work out as more expecnsive than buses so if you are planning to stay for a longer period consider buying yourself a bike to get around.

If you're looking to travel further afield, Tel Aviv University has a train station adjacent to campus. You can see on the map that the train network gives you access to all kinds of interesting places in Israel such as Jerusalem or Haifa. You can use the train to get into Tel Aviv too in case the weather is bad!

To the south of campus you may notice there is quite a large and beautiful park called Hayarkon Park. Here there is a small themepark, lots of nice space and nature, including a cactus garden and so on- it is definitely worth a visit on a nice day! Unfortunately between the university and the park is a rather large highway, If you are cycling or on a scooter there is a bridge to use as an overpass or if you are walking you can also use the train station as an underpass.

It's important to note that in Israel the shabbath (or day of rest) takes place from Friday evening to Saturday evening. This affects the opening times of a lot of shops and also, importantly, the university train station will be closed. Not only does this mean you can not catch a train, it also means you can't use the underpass to walk to the park, so please plan accordingly.

2.3 OUTSIDE TEL AVIV
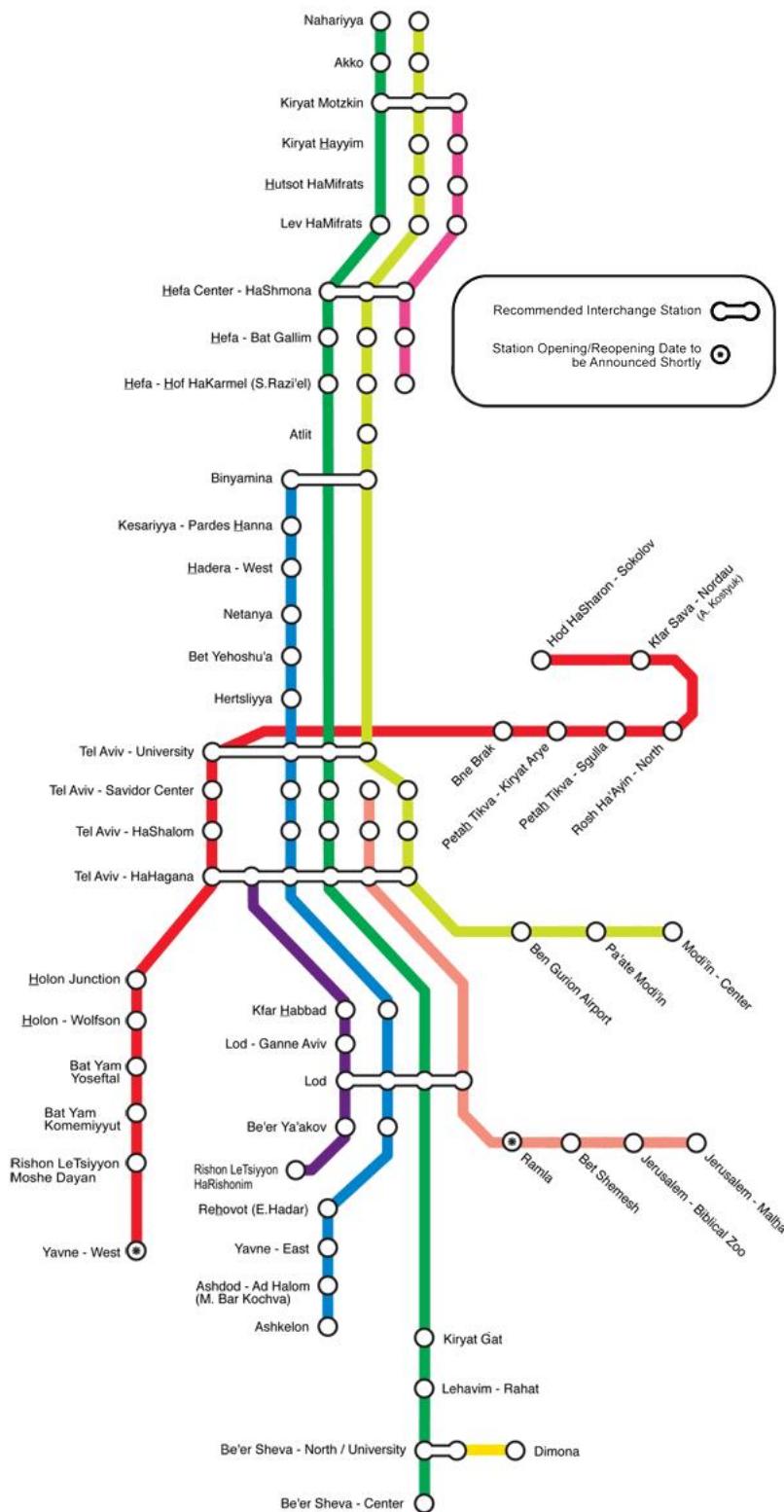
There are many obvious attractions in Israel outside of Tel Aviv, such as the Jerusalem or Haifa. I just take the time here to mention a few that are not so obvious and relatively nearby.

Akko is a historic and beautiful old town that is definitely worth a visit. You can see it is on the trainline to the north or there are busses fairly regularly as well. I won't say too much because it is something that should be experienced first hand but it is the site of an ancient Templar fortress as well as a bustling old market town. If you are looking for a simple day out, this comes highly recommended.

A destination that is also quite amazing is the Dead Sea. The best way to get here is to rent a car or find an Israeli friend who drives however, so it is not so straightforward as other destinations.

Note

Emergency service phone numbers in Israel are: a) Police 100 b) Ambulance 101 c) Fire 102

However, those who make it here will be rewarded with an amazingly unique experience of being at literally the lowest altitude on earth and the ability to float effortlessly in one of the saltiest bodies of water anywhere. In the height of summer it can get very hot however so plan accordingly.

Nahariyya

Akko

Kiryat Motzkin

Kiryat Hayyim

Hutsot HaMifrats

Lev HaMifrats

Hefa Center - HaShmona

Hefa - Bat Gallim

Hefa - Hof HaKarmel (S.Razi'el)

Atlit

Binyamina

Kesariyya - Pardes Hanna

Hadera - West

Netanya

Bet Yehoshu'a

Hertsliyya

Tel Aviv - University

Tel Aviv - Savidor Center

Tel Aviv - HaShalom

Tel Aviv - HaHagana

Holon Junction

Holon - Wolfson

Bat Yam Yoseftal

Bat Yam Komemiyyut

Rishon LeTsiyyon Moshe Dayan

Yavne - West

Kfar Habbad

Lod - Ganne Aviv

Lod

Be'er Ya'akov

Rishon LeTsiyyon HaRishonim

Rehovot (E.Hadar)

Yavne - East

Ashdod - Ad Halom (M. Bar Kochva)

Ashkelon

Hod HaSharon - Sokolov

Kfar Sava - Nordau (A. Kostyuk)

Bne Brak

Petah Tikva - Kiryat Arye

Petah Tikva - Sgulla

Rosh Ha'Ayin - North

Ben Gurion Airport

Pa'ate Modi'in

Modi'in - Center

Ramla

Bet Shemesh

Jerusalem - Malha

Jerusalem - Biblical Zoo

Kiryat Gat

Lehavim - Rahat

Be'er Sheva - North / University

Dimona

Be'er Sheva - Center

Recommended Interchange Station

Station Opening/Reopening Date to be Announced Shortly

3 GROUP

Welcome to Burton Materials Data Lab! We hope you have a productive and rewarding time with us.

I've worked in 9 different research groups in 6 different countries and I've found cooperation and teamwork to be the most important factors behind successful research. Surprisingly though, it seems almost no one talks or writes about it. Perhaps most of this section will seem obvious to some people but since we are an international collective I think it's worth writing it down so we all understand each other.

3.1 YOUR COLLEAGUES

Ultimately, this group exists to produce internationally significant research. Even if you do not aspire to an academic career, the kind of outputs we aim to create will be of great benefit to you in the future. Almost all jobs will appreciate proof of the following:

- professional writing
- international languages
- public speaking
- numerical literacy

- data handling
- team work
- time management
- effective administration

As scientists we should also be open to new experiences. If you are interested in alternate outputs for your time in our group please speak to me. For example, if you wish to create video's, websites, graphics, blogs, give public talks or any other form of science outreach I'd be happy to support you as much as I can. These can then be mentioned in a recommendation letter to future employers.

We should all commit to helping each other regardless of long term goals or how much time you intend to spend in the group. That way individuals benefit from evidence of professional development and the group benefits from being better established in the international research community. These effects enhance each other in turn, multiplying our collective success.
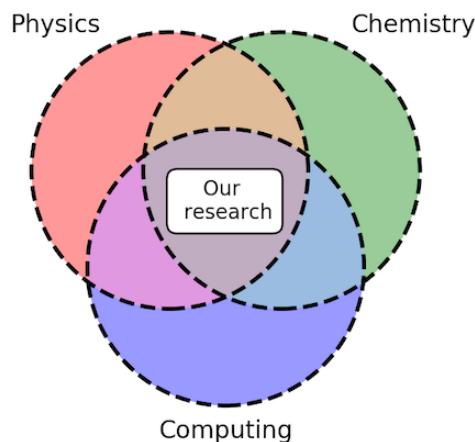
Everyone should be constantly learning as they work. Try to always have a notebook to hand so that you can draw or quickly write

> **Note**
>
> Angela Merkel has a PhD in quantum chemistry. She became the first female chancellor of Germany and was described as the most powerful woman in the world. The qualifications & skills you can obtain with us can be useful in any career path, not just science.

down paper details whenever they may come up. The physics of the methods, the chemistry

of the materials and the data science of the code packages all overlap in our area of research, as shown in the Venn diagram below. No one person can understand all of these 3 areas, as they are individually developing rapidly in different directions. It is important that we are honest with each other if we do not understand something, there is no shame in asking for help. However, adjusting numbers, altering figures or hiding errors will in no way be tolerated from anyone. If you are unsure, just ask :)

Safety is incredibly important for a shared work space. Do not run wires across areas where people can trip and make sure to clean up any spills before someone can slip. If you must stay late at night, try not to be the only person in your office: if you fall and no one is around to help you, even a minor incident can become a major problem. There will be a minimum standard of cleanliness expected of everyone. We also share quite a lot of space with other groups so please be considerate. That said, I encourage you to decorate your desk and office space in whatever way makes you feel comfortable.

I want to specifically try and bring together students from different backgrounds but with complementary skill sets. This might mean you don't feel that you have a lot in common with other group members. For this reason, I will regularly suggest we go for dinner or perform an activity that is not work related. This will help people discover mutual interests from different perspectives and get to know each other better on a personal level.

Finally, always try to be kind to each other. Bullying, harassment or treating anyone differently because of their gender, origin or appearance will not be tolerated. Every member will treat every other member equally, with respect and professionalism. This extends to any guests, visitors or support staff you encounter. If you have an issue with another individual, first try explaining to them that you are not comfortable with their behaviour. If the issue persists, please bring it to my attention.

Note

Richard Feynman famously said "if you think you understand quantum mechanics, you don't understand quantum mechanics." This is just one of many topics we need to be familiar with, so don't feel bad if you don't understand everything.

Research has to be challenging. If you think a project is easy that's because you are not pushing yourself. Science exists as a series of increasingly difficult models, from the cartoons you were taught as a child right up to the physical reality that is impossible to understand.[1] Where you fall on this scale depends on your level of training but if you are finding research easy you need to consider moving to a higher, more sophisticated level. Conversely, if you are finding research too difficult you can move one stage back until you feel you are ready to move forward again.
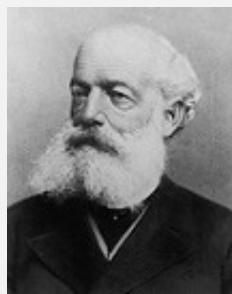
However, just because research must be difficult doesn't mean it has to make you miserable. I had a fantastic time during my early research career and I hope I can help you to do so too. Happy people are more productive and creative,[2,3,4,5,6] which are the 2 most important skills in research. Happy people are also nicer to be around, increasing the chance of having interesting discussions and establishing collaborations. So it is really to everyone's benefit that you are happy in your research!

Happiness is greater in more scenic environments,[7] and we are lucky to have a beautiful campus right outside. In England it is so rarely hot and sunny that people don't think twice about leaving the office when the weather is nice. As long as people can reach you, *via* Whatsapp for example, and we have no meetings scheduled then feel free to enjoy the beautiful scenery around Tel Aviv.

> **Note**
>
> In 1865 August Kekulé famously deduced the structure of Benzene based on a dream of monkeys dancing together. Sleep and rest have long been associated with effective problem solving!

I will always try to offer a selection of projects from which you can choose the one you would prefer to undertake. Think carefully about the one that motivates you most on a personal level. Things won't always go perfectly to plan, so believing in what you're trying to accomplish in the project can really help you stay motivated. I can think of almost no scientific reason why a project would need to be abandoned. Even if someone else publishes your exact project before you do, it can still be published and is valid as a body of work itself. If you are really having trouble, please talk to me but don't just try to switch projects because it's not as much fun as you first thought.

Manage your time and health properly. Working long hours has been shown to be bad for

---

[1] P. W. Anderson, Science, vol. 177, no. 4047, pp. 393-396, 1972.

[2] A. M. Isen *et al.* Journal of Personality and Social Psychology, vol. 6, no. 52, pp. 1122–1131, 1987.

[3] F. G. Ashby *et al.* Psychological Review, vol. 3, no. 106, pp. 529–550, 1999.

[4] B. L. Fredrickson, Philos. Trans. R. Soc. Lond., vol. 359, no. 1449, pp. 1367–1378, 2004.

[5] A. K. Anderson *et al.* Proceedings of the National Academy of Sciences, vol. 103, no. 5, pp. 1599–1604, 2006.

[6] G. Rowe *et al.* PNAS, vol. 1, no. 104, pp. 383–388, 2007.

[7] C. I. Seresinhe *et al.* Scientific Reports, vol. 9, no. 1, p. 4498, 2019.
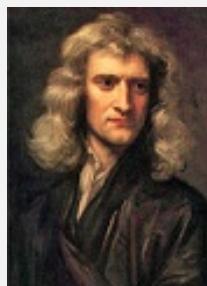
your body,[8] and your mind.[9] Even in the short-term working long hours can be unhelpful. You will certainly be more productive working for 4 hours after an 8-hour sleep than you will working for the same 12 hours with no sleep.[10] Do not think I will be impressed to find you in the office late at night or asleep under your desk in the morning. There also is the danger of undoing good work that has already been done. I once accidentally deleted the entire headnode of a super computer that hadn't been backed-up for 3 days. I promise you that every single user of that computer would prefer I had stayed in bed that day rather than go to work!

It has been shown that researchers had very high incidences of poor mental health compared to other professions.[11] The Institute Of Physics (IOP) has published a 40-page guide to building and maintaining well-being for researchers in physics,[12] so while I don't discuss self-care any further in this guide, there is a lot more to this than what I've written. I will make the IOP guide available along with this one.

Note

Isaac Newton discovered gravity after an apple fell on his head. He was sat outside, in a garden, under a tree. Your frame of mind in conducting research is more important than sitting in the office all day.

Increasingly, companies in Europe, America and Australasia are moving towards a 4 day week because it has been shown that taking fewer holidays is linked to poor health.[13] Google doesn't implement a 4 day work week but they have a policy that is similar. It is called the 20 % time rule, and you can hear the former CEO of Google talk about it yourself.[14] This is a rule that employees should spend 1/5th of their time (i.e. one day out of 5) working on something unrelated to their specific job. Back when this idea first became famous, a lot of people thought it was stupid and wouldn't last, however the company has gone from strength to strength and, even now, they still win the title of most innovative company. [15] I'm happy working 5 days of the week and I don't expect you to work more than that. I also don't expect to see you in the office all of the time. If you study and write while at home with you parents it still counts as work done.

If you are ever sick, please do NOT come to the office. I know some people think that this is a display of commitment to their work but I really don't. I don't want your illness and nor does anybody else. If you need time off, take time off. Similarly, if you are not sick but need to stay home because of, for example, a sports injury or pregnancy, it is possible for you to accomplish work while outside of the office. We can arrange Zoom meetings or alternatives so

---

[8]Virtanen M *et al.* American Journal of Epidemiology, vol. 1, no. 7, pp. 586, 2012.

[9]Virtanen M, *et al.* PLoS One 7, 1 2012

[10]M. Björnmalm, Science, doi:10.1126/science.caredit.aax5716

[11]"The mental health of PhD researchers demands urgent attention," Nature, vol. 575, pp. 257-258, 2019

[12]S. Shinton, "Resilience Toolkit: A Physicist's Guide to Building and Maintaining Wellbeing", Institute of Physics, 2019.

[13]T.E. Strandberg *et al.* European Geriatric Medicine, vol. 8, no. 3, p. 260, 2017.

[14]https://mashable.com/2018/05/11/google-20-percent-rule/#OuoJO9zf5kqU

[15]https://which-50.com/google-not-apple-named-bcgs-most-innovative-company-in-2019

that progress in your research can still be made. However, overall you will be most productive on campus and, if you are able to do so, please try to be around between 10am-4pm.

> **Note**
>
> I've been told that my ideas are western but Confucius said 'To put the world in order... we must first cultivate our personal life.' Taking care of yourself makes sense, no matter where you are from.

Finally, money is important to everyone but scientists rarely talk about it. There is unfortunately very little money in science for students but I strongly believe that science should not just be available to students from wealthy families. If you need to get a job, I will not consider it a demerit. I already said I won't expect to see you outside of a 10am-4pm, Monday to Friday. In theory this leaves time for you to work evenings and weekends. I advise working a second job no more than 3 or 4 days each week, but this decision ultimately must be made by you.

There are opportunities available in the university and even our research centre where you can earn a little extra money. I think this is the most ideal way to do some work on the side, as it won't distract you too much from your research and you don't have to spend time travelling between different jobs *etc.* The best way is to talk to me and we can try and organise something based on your specific requirements.

3.3 Your Supervisor (Me)

As far as you are concerned my only job is to support you; so you never have any reason to lie to me or hide from me. 99 % of the time our relationship will only be work related but that doesn't mean you can't talk to me about other issues in your life. If your house burns down in the middle of the night and you have no-where to go, you absolutely *should* contact me. Just because it is not work related doesn't mean I can't help you.

In the past I have worked with people who had suffered brain damage, were HIV positive, and had recently lost children. No matter what your issue you will not surprise me BUT please understand that I am not a trained therapist. I will support you as much as I can but most of the time this can only extend to providing you free time to seek alternate help or to help yourself.

I will correct your spoken English, especially if there is scope for confusion in what you said. This is never intended to humiliate you, but small corrections over the years spent studying a masters or PhD can add up to a professional level spoken English by the time you graduate. I know this from my time spent working in in Belgium, Japan and China.

I've tried to encourage you to be creative but this doesn't help us if we never discuss your thoughts. Everyone should feel free to approach me with project ideas whenever they are ready. In principle coming up with a project is easy. You can simply follow the framework: Component -> Class -> Application -> Method. Any combination of suitable words or phrases can be thrown together in this way to make a reasonable sounding project, for example "Aluminium alloys for the construction industry by structure prediction" or "Titanium perovskites for water-splitting
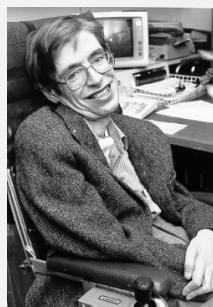
by machine learning." etc. However, just because it has a sciency title doesn't mean it's a project worth pursuing!

In Europe it is possible to obtain a PhD having published no papers and so they are more able to take on 'risky' projects. Here, we do not have this luxury so we have to be extra careful when thinking about starting new projects. While I encourage everyone in the group to cultivate project ideas please don't feel dejected if we don't decide to pursue it. Before a project can start there needs to be consideration of the

> **Note**
>
> Stephen Hawking was diagnosed with Motor-Neuron Disease at 21. Most people might have thought this the end of his work but he went on to have a long and productive career because he received the right support.

literature and activity in the field to know which are the most feasible. Things to consider include: do the tools already exist to perform these projects or would we need to create our own? Would this study be of interest to the community even if the results are negative? Is there someone we know who we could ask to collaborate with us?

It's an unfortunate truth that I will need more help from you than an Israeli supervisors will need from their students. Even small tasks can be quite difficult in another language. It also means that you cannot always rely on me to warn you of arbitrary things like paperwork deadlines. I already heard of one student missing out on a PhD scholarship because their (foreign) supervisor didn't know about an early deadline. If you ever hear me say something that you think is wrong you MUST correct me. This applies for science as well as administration.

Finally, I will keep a calendar that is up to date, and available for you to see. This means you can know when I'm busy and when I'm not - so if I have an upcoming work trip, for example, you might want to speak to me before I leave. This is better than me announcing where I'm going to be all the time. You are free to add your own work-related events in to the calendar so that I know when I can find you too, but this is not required. Furthermore, if you see that I am or someone else is participating in something you might be interested in, then you can always ask to join too.

4 WORK

Research and studying are both necessary in academia; studying is time spent acquiring new knowledge, (*i.e.* reading papers) while research is time spent applying that knowledge to create new results (*i.e.* running calculations). If you only do research and never study, you will not succeed academically because you won't know how your results fit with modern technology and society. Similarly, if you only study and never do research you will also not succeed because you will never contribute to the community. The balance between these two things ultimately depends on the person and the project, so resist the urge to compare yourself to others.

> **Note**
>
> Cecilia Payne was the first person to discover what stars are made of but was discouraged when nobody believed her. She described her results as spurious at the time but regretted it later saying: "If you are sure of the facts, you should defend your position."

One should start a project by studying what has already been done, so I begin this section with a guide to understanding the literature. Then I discuss some basic details for performing research with software that is already available. Finally, I discuss managing data, that is to say making sure the data is clear and available to the point that you and others can spot anomalies, errors or interesting trends even after your work is published. Your contribution to science should long outlive your stay in our group, managing the data is crucial to achieving a lasting impact.

4.1 UNDERSTANDING EXISTING RESEARCH

4.1.1 PAPERS

Research papers are published in journals. Usually, different journals cover different topics. However, there are different journals that cover the same topic, and these usually fight between each other to be considered better. How good a journal can be considered is usually measured with an impact factor, which is updated every year. It's a metric derived from the average number of citations of papers published by this journal. It should in no way be considered as a indication of trustworthiness for a study. There are bad papers in very highly esteemed journals and good papers in relatively obscure journals. Our training as scientists always takes priority over such simple metrics.

Journals can have subcategories of themselves. For example the Journal of Materials Chemistry is split into A, B and C. These are not grades of quality or merit, simply distinct topics. Here, the Journal of Materials Chemistry A is for research in materials for energy and sustainability; B is for research related to biology and medicine; and C is for research related to optical, magnetic and electronic materials.

There are also journals that aim to cover ALL topics- you may have heard of the journals Nature and Science. These journals concern themselves with 'breakthroughs' in research, and are usually written and read very differently from more specific journal articles.

Each journal can have different types of publication:

- Research article. This is the standard publication format for a research project. it is the primary vehicle by which results are disseminated.

- Review. This is a publication in which one or a few authors try to summarise progress in an entire field of research.

- Perspective. This is a publication in which an author talks about their own research, usually over a long time frame.

- Editorial. This is an endorsement of another research groups publication in a relatively casual format. These exist because research papers can be quite difficult to understand or follow if you are not immediately familiar with a research area.

- Commentary. A commentary is an opinion on a topic or area of research. They are written at a level accessible to readers who are not researchers themselves but who are interested in research.

- Erratum. An erratum (sometimes called a corrigendum) is a paper published to highlight a mistake in a previous paper by the same authors.

There is an enormous difference between these types of paper. You need to understand these differences so that you can better judge the literature. For example, if you find a research article that makes a conclusion and a commentary that states the opposite conclusion, this is not a 50:50 split in the literature. The article should be given more weight in your consideration because it is a study, whereas the commentary is an opinion.

Each Journal is made by a publisher and each publisher has several journals. This can be a little confusing because, for example, the journal Nature is published by the publisher Nature. Some people have strong feelings about the distinct publishing groups because some of them are not-for-profit and some of them are very much for profit.

Understanding the difference between journals and publishers, and the types of articles on-line, empowers you to better judge the field. It is an unfortunate fact that people do try to misrepresent this information. The most common misrepresentation of this information I've seen is for the journal Scientific Reports, published by Nature. This journal was created to

accept any research paper that is scientifically valid, no matter perceived importance. The Journal Nature published by Nature on the other hand only accepts what is perceived to be the most exciting and impactful research in the world. As you can see, these two journals by the same publisher have an enormous difference in impact on average. However, more times than I can count, I've seen people reference their own work published in Scientific Reports and try to imply it is published in Nature... do not be fooled!

4.1.2 PREPRINTS

A problem that existed for a long time in science is that it is possible for someone else to publish a result before you, even though your paper was submitted first. The peer-review and editorial process can be quite arbitrary, sometimes getting published quickly, other times taking months.

A solution to this came in the form of a website called arXiv (pronounced "archive") which acted as a place to upload your work before submitting it to a journal. Such a thing is called a pre-print and has no pay-wall or access restrictions for potential readers. This allows scientists to lay claim to a result or discovery as soon as a coher-

Note

Henry Ford was very important in the development of mass production, but he didn't patent a single tool or process! While we may try to create patents for some projects, do not feel left out if there are not similar opportunities in your work. All research has merit.

ent paper has been put together rather than when a journal deems your work worthy of publication.
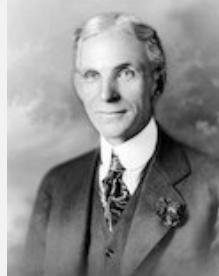
The use of pre-prints divided the research community originally with most journals refusing to publish an article already on arXiv. Increasingly however they are being used, with new repositories such as ChemArXiv (chemistry archive) and BioArXiv (biology archive) appearing recently. Their use has even increased to the point that some people claim that journal publications are no longer necessary.

4.1.3 PATENTS

A patent is legal ownership of an idea or technology. If you discover something first and patent it, companies/universities must seek your permission before using your discovery.

However, during the process of a patent application, clerks will search through all previous discoveries and publications to check if you really are the first to make this discovery. If you have ever revealed information publicly about your invention, it can then never subsequently be patented. This includes everything from a presentation at a big conferences, right down to a tweet or facebook post.

Our group will always strive to make our work available to everyone where-ever possible. For example, this guide can be read by anyone on-line. However, when it comes to scientific research, it is better to keep that information within the group until the results are under peer-review or already published. Even if you have no plan to file for a patent, a journal usually won't consider publishing works already available elsewhere. Please do not post your results to social media and certainly never post somebody else's information on-line.
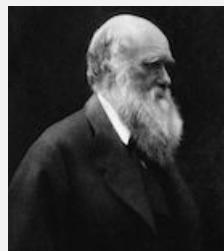
As part of a patent application it must be proven to exist. For theorists, that means we must collaborate with experimentalists to prove our predictions. No country will let you patent something based on a DFT prediction, unfortunately for us! Luckily there are a lot of amazing experimental scientists who are happy to collaborate, especially when it can lead to a patent.

4.1.4 LEADERS IN THE FIELD

An important thing to know for a successful time working in research is who are the leaders of the field. These are the people doing good work we should follow outside of Tel Aviv. If you go to a conference these are the names you'll hear people speak about and it can help a lot to have a general understanding of what they do in the field. These days there are also tools like Twitter and Google alerts that allow you to keep in touch with or follow the work of these groups all year round.

In a lot of cases it's not possible to compete with these leaders directly because they have longer academic experience and therefore deeper knowledge. They are also likely to have larger groups, or more money, or alternate expertise or a combination of all of these. This does not mean they are enemies or that we have anything to worry about. There is an infinite amount of research to be done, we just want to make sure we're using our time effectively.

Note

"It is the long history of humankind (and animal kind, too) that those who learned to collaborate and improvise most effectively have prevailed." – Charles Darwin

- Materials Project/Pymatgen:
  - Gerbrand Ceder, University of California, Berkeley, USA.
  - Kristin Persson, Lawrence Berkeley National Laboratory, USA.
  - Anubhav Jain, Lawrence Berkeley National Laboratory, USA.

- Materials Theory:
  - Chris van der Walle, University of California, Santa Barbara, USA.
  - Fumyasu Oba and Yu Kumagai, Tokyo Institute of Technology, Japan.
  - David Vanberbilt, Rutgers University, USA.

- Experimentalists:
    - Hideo Hosono, Tokyo Institute of Technology, Japan.
    - Andriy Zakutayev, National Renewable Energy Laboratory, USA.

- Materials Modelling:
    - Suhai Wei, Beijing Computational Science Research Center, China.
    - Alex Zunger, University of Colorado, USA.
    - Aron Walsh, Imperial College London, UK.
    - David Scanlon, University College London, UK.
    - Nicola Marzari, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland.

- VASP:
    - Georg Kresse, University of Vienna, Austria.

- FHI-AIMS
    - Volker Blum, Duke University, USA.
    - Matthias Scheffler. Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany.

This is not everyone doing good work in materials science. You will find that depending on your specific topic you will hear certain names repeatedly and see them recurring on your favourite papers. There is no such thing as absolute science, and the human element is important for all research. Learn these names, contact people, speak to colleagues and you will find a sense of community in research and establish your own identity within that community.

4.2 PERFORMING NEW RESEARCH

Everybody has a research project that is unique to them. I don't try and cover the science in this guide, there are textbooks available for that. What I want to describe here is a framework that can allow anyone to perform their own research, even as it changes over the course of a project.

Note

According to Maria Goeppert-Mayer "Winning the [physics Nobel Prize] wasn't half as exciting as doing the work itself". If you choose to work on something you are passionate about you don't need awards or recognition to stay motivated.

Virtually everything we do will take place on a computer, even reading papers is almost exclusively done electronically. I will try hard to maintain a computer structure that allows all of us to create accurate and reliable results. It's

Note

Oliver Heaviside worked with physical concepts before they were formally proven. When asked why, he said "Shall I refuse my dinner because I do not fully understand the process of digestion?" You too shouldn't wait to understand all aspects of VASP before you use it.

important that we keep on top of the tools that we use, which other tools they interact with and what they require to work so that we don't get swamped with competing codes from all over the internet. This framework will naturally change over time and if you have any suggestions for change you are more than welcome to make them.

Having a recommended framework of computer codes offers several benefits. Firstly, we can develop a deeper understanding of an individual tool as a group, rather than try to keep track of multiple implementations of the same theory in similar codes. Secondly, it may be necessary to write codes that wrap around specific tools, either to process the output or generate input files etc. These wrappers can be more easily shared, developed and used by the whole group if there are fewer to work with. Finally, it is inevitable that we will have young students start with us who are keen to contribute to our research. If we have specified tools for common outputs, then even the newest students can begin creating impactful research that is consistent with previously generated results without necessarily understanding all of the theory behind it (of course, everyone is strongly encouraged to study any methods they use as their research progresses).

The one drawback that comes with relying on only one code for each output/property is that if there is a bug in that implementation then we may not be aware of it because we are not comparing across multiple codes. We must always be on the lookout for strange and unusual behaviour from our simulations, which is where our understanding of materials science becomes crucial.

4.2.1 Your Computer

You are welcome to install or access any software you feel will support your research and learning but please also install the following tools that will help us work together.

4.2.1.1 Latex: The end goal of any project is a paper, report, or document that describes your research. It is likely that when you start in the group you may only be familiar with Microsoft Word. This is totally understandable and widely used the world over. You can continue to use this for as long as necessary, but it is strongly encouraged that you begin to teach yourself LaTex to make professional PDF documents as soon as possible, especially, if you are writing a PhD thesis. I wrote my PhD thesis not that long ago and almost everyone in

my graduate school who chose to write their thesis in Word encountered problems eventually. Word is fine when your documents are a few pages long but when you are looking at making 150+ pages including, cross-referenced figures, tables, citations, equations and all the rest, it quickly becomes unmanageable.

LaTeX also allows for the use of templates and standard formats. This means we can create and maintain group templates for masters and PhD theses and other document types. Of course, you are welcome to modify your own document as you wish, but for the most part, having a minimum standard of quality and clarity will significantly simplify the process of thesis writing, and help minimize stress towards the end of your project.

4.2.1.2 ANACONDA: Anaconda is a tool to create virtual environments, which are like smaller computers within your computer. The reason this is useful is that it can create an area that is standard for programs, whether you are using windows, apple or linux machine. Because of this a lot of research code writers develop their codes for use within anaconda and in some cases even use anaconda as a platform for distribution. It's also useful for us to work inside virtual environments because if you make a mistake and break a code or cause a software error, we can simply reset the environment. If you do something damaging and it's not inside an environment you can cause serious harm to your computer and lose work.

Note

Max Planck said "we see in all modern scientific advances that the solution of one problem only unveils the mystery of another". At some point we have to stop and say, this level of theory is enough to describe what we seek.

4.2.2 THE CENTRAL COMPUTER (POWER)

Calculations can require a long time and a lot of computing power. For this reason we have a very powerful central computer that is hosted by the Tel Aviv University Computing Center. This computer, usually called a cluster because it is a connection of many different parts, is optimised for running these difficult calculations all day every day. It's possible to find software to interact with this computer in a similar way to your own computer, and I encourage you to use these in the beginning. For example, WinSCP lets you drag and drop files between your computer and the cluster. However it's faster, easier *and* more powerful to use command-line prompts, which in this case will be in the programming language Bash. To learn more about Bash and how to use it from any operating system, please see the online tutorial we have written for new users.[16]

---

[16]https://github.com/bmd-lab/tutorials

4.2.2.1 VASP: VASP stands for Vienna Ab Initio Simulation Package and it is the tool we use to turn atomic structure into materials properties. It is not the only package that can do this and it is certainly not perfect (I wouldn't even say it is the best available). The reason I, and many others, choose to use VASP for re-

search is that is fast and easy to use, this means the barrier to entry is low for students and researchers outside of quantum physics. Other *ab initio* packages like VASP include but are not limited to Quantum Espresso, CASTEP, ABINIT and GPAW.

When you are a little more familiar with coding, there are ways to generate the files for VASP automatically. In the beginning its best for you to play around with the files yourself so that you understand better the machinery of your research. The absolute minimum you need to know to run a calculation is that there are 3 files you must prepare INCAR, POSCAR and POTCAR. These files are so named because a long time ago computers used to be given information on punch-cards. So INCAR- comes from INput CARd, POSCAR comes from POSitions CARd and POTCAR is POTential energy CARd.

A basic INCAR contains the option flags for the calculation and will look like this:
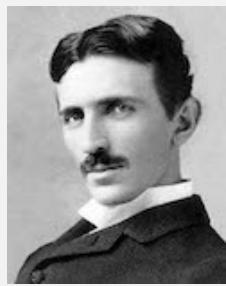
```
INCAR

 ISIF = 3                #Allows structure to relax to its lowest energy


 IBRION = 2              #Sets method to optimise relaxation


 NSW = 100               #The maximum number of ionic steps.


 ISMEAR = -5             #Sets treatment for partial occupancies orbitals
```

VASP will run a calculation with this INCAR but you should know there are more than 300 options that can be set in this file! VASP has an on-line wiki that explains these features in more detail and is updated with the software. So for further details I'll refer you to the website. [17]

POSCAR is the file containing the atomic positions and is split in to three sections. First the repeating unit cell is defined as a 3 × 3 matrix, then the number of atoms is specified, finally the 3-D positions are listed individually as coordinates. The primitive cell of silicon looks like this:

---

[17]https://cms.mpi.univie.ac.at/wiki/index.php/The_VASP_Manual

```
POSCAR
Si2
1.0
        3.8669745922         0.0000000000         0.0000000000
        1.9334872961         3.3488982326         0.0000000000
        1.9334872961         1.1162994109         3.1573715331
    Si
     2
Direct
      0.750000000         0.750000000         0.750000000
      0.500000000         0.500000000         0.500000000
```

The line that says 'Direct' can either be this, which means the coordinates are relative to the unit cell or 'Cartesian' which means the coordinates are defined as absolute with respect to an origin.

Finally, a calculation needs a POTCAR file. VASP comes with a POTCAR file for each element and you just need to bring the files for the elements of your system together for the calculation. Be careful because the order of the elements needs to match the order you specify them in the POSCAR. I heard of one student who found out at the end of her project that the POTCAR was in the incorrect order, making all of her conclusions incorrect.

These three files need to be in a folder together to run the calculation, there can be other files in there too but i recommend each folders be kept clear of anything except the relevant calculation files.

4.2.3 EXTERNAL RESOURCES

4.2.3.1 PYTHON: Python is a powerful, human-readable, free and very popular programming language. It is not automatically distributed with linux or windows, nor is it strictly necessary to perform calculations, so here I consider it an external resource. However it is free, so if you are comfortable with the tools described in the previous section you should consider installing python.

Python is the language with which we will do most of our science. Equations, data manipulation, conversions, graph plotting *etc.* are all much more suited to python than the other languages we've talked about. Python can be thought of as a free and open-source equivalent of MATLAB, with which you may be familiar.

Python is also a command that you can use from the terminal. If you type python by itself the computer will begin a session in which python is now the language rather than BASH. If you type python and then a file written in python, the computer will execute that file.

I won't try to teach you python here, but i recommend the website code-academy as a resource that I think is quite universal for students in the field.

4.2.3.2 PYMATGEN/MATERIALS PROJECT The Material's Project is a database of many thousands of materials that have already been simulated with VASP. Even if you are not looking to
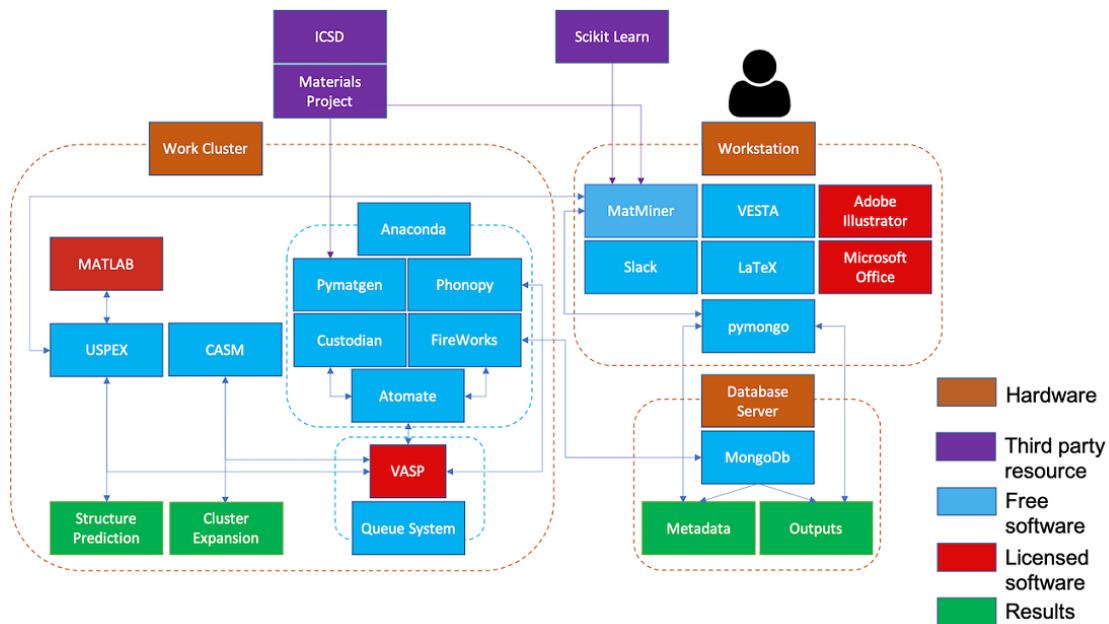
Figure 4.1: A schematic of the ideal software infrastructure. Each box indicates a code, package or computer and the arrows indicate with which other code they interact.

directly interact with the Materials Project it has become an important point of reference for scientists in our field. If you calculate a band gap of of 3 eV but the Materials Project shows the same material has a band gap of 0.9 eV, we need to check if something went wrong.

As your skill grows you will be able to use python to access the data within the materials project directly using a library called Pymatgen (short for PYthon MATerials Genomics). This is the stage at which high-throughput studies become available to you. High-throughput by definition means consistent analysis of many thousands of systems and for us, it is with the Materials Project and pymatgen that we can do this.

> **Note**
>
> Marie Curie was Polish but worked in France. She said, 'science is essentially international, and it is only through lack of historical sense that national qualities have been attributed to it'. The internet is a powerful resource to connect us to the globe - we must use it.

4.2.4 SUMMARY

I've talked about the bare-minimum in this guide but you should know there are a lot more tools out there that we use as a community and many of these interact with or even depend on

each other. The best pictographic representation of a overall infrastructure for the group that I've been able to come up with is shown in Figure 4.1. You will probably only use part of this work flow so don't worry about keeping on top of everything.

4.3 Managing Data

Once you are at the stage of high-throughput analysis or automating calculations with coding, it is easy to generate massive amounts of data over the course of a project. It is important that we manage our outputs properly or we will be out of storage space in no time. This can be as simple as NOT outputting wavefunctions and charge densities from calculations where they are not needed, but certainly we must be careful to not delete data we rely upon in drawing later conclusions.

This is especially true because we also need to keep track of our metadata. 'Data' are the results from your research, but metadata is the information related to these results. For example, the results file is data, whereas the location of the results file is metadata. Metadata includes but is not limited to: date, file size, file ownership and permissions *etc.*

As an example of this, I once found that the total energy for a calculation was slightly different depending on the number of cores over which I parallelised the calculation. In theory this should have made no difference, and I use it as an example because almost no one records the number of cores over which a calculation is run. In the end it turned out to be such a small difference as to not affect the results of the study overall, but we should still try to record as much information about our work as possible so that we can trace back any unexpected issues.

Note

I'm not the first to see the importance of creativity in research. Ada Lovelace said 'Imagination is the discovering faculty, pre-eminently. It is that which penetrates into the unseen worlds around us, the worlds of science'

My suggestion for dealing with this is as follows. Each potential research paper should be a folder on your computer. Any result that you present in the paper should have the corresponding calculation from which that result came in said directory. Once the paper is published (AFTER all of the peer review etc), compress the directory with all of the relevant calculations in it (and perhaps a little plain text explanation) with the 7-zip method. This is a very thorough compression that takes a long time but allows for a large reduction in size. We'll have a central, backed-up storage for keeping these, and then you can clear out the calculations for that project and free up some space. This kind of data preservation is not only good practice but usually a required condition for research funding so please take care with this.

4.3.1 Github

Hopefully, you've seen how programming languages can be powerful and stored conveniently as files. Once one of these files becomes more than a few lines long it is now a code. Codes can become complicated very quickly, sometimes even you can break your own code trying to incorporate changes (this happens to me lot!). 3rd party services exist to help track changes, include documentation and update safely any code you are working on. Github is one such service that is very popular and also free for academic use, luckily for us!

Github allows you to do all of this for your code in either a private way or open to the internet. Using github just by yourself is still useful. As it highlights some of the best practices for coding. If you have 3 things you want to fix in a code, don't try and fix them all at the same time. Fix one, then push to git. Then fix the second, check the first still works, then push to git. Finally fix the third, check the first and second, then push to git. If something goes wrong, you can use Github to revert to a previous version of the code with no harm done. It also has commands such as 'git status', which is very useful. It lets you see the difference between the files on your computer and the files of the last upload to Github.

The biggest use of github however is with the open (not private) repositories. Scientists recognise that there is great benefit to opening their work to the community *via* the internet, as I said earlier, you should never try to do everything yourself. However, you can't simply allow anyone to edit your codes as they please or they could introduce errors, change the way you wanted it to work or break the code entirely.

You upload your code to Github and people can 'pull' the code to their computer and 'push' changes for you to consider. If you don't like the changes you can reject them, but if you do approve you can accept.

Github can get a little complicated as codes can be branched and merged. One code can have several

> **Note**
>
>
>
> Don't be discouraged if you didn't study a topic. J. Oppenheimer (father of the atomic bomb) once said "there are children playing in the street who could solve some of my top problems in physics". Fresh insight is invaluable in research!

branches, each with different versions to the main branch. This kind of complexity is usually only encountered for very popular or ambitious codes however, so you don't need to worry about such things in the beginning.

5 OUTPUTS

This section is dedicated to creating impactful research outputs from your understanding of the field and new results. In theory, there is no limit to the ways you can share good science with society, but there are unfortunately only a few ways you can do so and receive official recognition.

5.1 ARTICLES

The formats of research articles vary depending on the journal we will submit to. It can be frustrating because if the paper is rejected it might need entirely reformatting before submitting to the next journal. However, regardless of which journal we submit to, you should have a master-draft article containing the following sections: Abstract, Introduction, Methods, Results, Discussion, Conclusion.

I recommend that you start collecting pertinent data from the very beginning of the project. The first few weeks of any new project should be spent reading the literature. Similarly, any document should begin with a literature review. Take the opportunity to note your thoughts and impressions as you read in a LaTeX document. Do you spot any conflicts in the literature, are there any ideas that everyone seems to agree upon, what is the range of values you see reported for the same materials property? I find a useful exercise is to see how far back you can trace the topic of your study. How have things changed since then? Before you know it, you will have a Literature Review on your hands.

Any time a calculation finishes, put the result of that calculation in a document along with the method you used and where you stored it. I guarantee there will be times where you forget from where you got a specific number. Under no circumstances can we publish results that we can't trace back to the completed calculation files. This may mean running calculations again if they are misplaced, so please be careful.

Note

Margaret Hamilton standing next to the software she and her team at MIT produced for NASA's Apollo Moon missions. This is an amazing feat of coordination, teamwork and data management... not to mention science!

Keep the calculation details in a document separately so that they can be added to as progress is made. The details should be a stand-alone, factual record of inputs and outputs. The inputs will form the methods section and the outputs will form the results section.

For a methods section there are also a few other rules you should follow. If you make any modifications to anything they must be described. If you use any software you should use the version number or release and if you write any wrappers or stand-alone codes yourself they should be made available along with the paper. Anybody should be able to sit down with

your paper, assemble the tools you used, follow your method and get the same results without having to access another paper.

There is no room for opinion in either of the methods or results sections, but as we start to see many different results side-by-side we can start to draw on our training as scientists to infer underlying physical phenomenon. This is what the discussion section is for and should include observations such as do all the results from the same method follow an obvious trend? Why do you think changing that one flag in the input file changed the result the way it did? Are there other materials that behave similar to this one?

Do not worry too much about your English. One of the benefits of a British supervisor is I can take care of that but its good for you to practice by yourself. No matter how bad you think a draft might be, do not EVER pay someone else to write an article or essay for you.

5.1.1 Authorship

It's very important that everyone receives credit for work they have done. If someone contributes to a project such that their result is included and they are the best person to explain it, they need to be an author. If their result or idea is included but no explanation is necessary, then it might be acceptable to simply credit them in acknowledgements. I've encountered a lot of strange ideas about authorship in the past but ultimately there is no diminished value of your work from sharing your name with others on a paper. Do NOT try to do all the work yourself to keep all the credit for a paper! I promise you your work will be of higher quality overall by involving specialists where needed. Finally, it's not possible to go back and add someone's name to a paper after publication and missing someone off a paper they worked on will generate an incredible amount of ill-will for the group from important collaborators and colleagues.

> **Note**
>
> Tu Youyou described her discovery of a Malaria treatment as "an example of successful collective effort" and cited the combination of chinese and western medicine. Not just different people but different cultures can lead to great discoveries!

Respect in the community may not seem immediately useful. But I know a scientist who, at the time of writing, has five publications in Nature sister journals that are all reviews, commentaries or perspectives entirely because their opinion is respected and their expertise recognised internationally. There's no way a group can elevate to this kind of status if they are known for shoddy work, falsified results or stealing credit!

5.1.2 Citing works

Pre-prints CAN be cited in your research but the exact wording or format of the document may have changed by the time it is published to a journal. The arXiv website won't always say

if a paper was published after being uploaded there but if possible you should cite the journal publication rather than the preprint. So make sure to search properly before citing a preprint.

I encourage you to cite text books as well as journals. In this way the time you spend studying the basic science can also bolster your research output.

The term DOI is an acronym of Digital Object Identifier. This is a tag or code that should always be used rather than a website url. Figshare, Zenodo and the preprint servers provide DOIs for citations, so its not just papers but also preprints, presentations and computer codes that have them. Usually when a code is released it is accompanied by a paper describing how it works. Most often this paper is the thing the authors would like you to cite if you use their code, but if you're not certain you can always cite both.

Copying from other published items (including your own!) is illegal. It is called plagiarism in English. While this means you can't copy sections or paragraphs I actively encourage you to copy lines from papers as long as you reference them properly. If you do not make any change to a line from another work by the time you come to publish it must be included as a quote but otherwise a citation is fine. Now more than ever its super easy to find if something has been copied from published work (even just using Baidu or Google) so don't waste our time by not citing properly.

5.1.3 SUBMISSION

Each article is written and submitted with a cover letter explaining why the study deserves to be published and why it was submitted to that journal in particular. The paper will then either be rejected based on the editors opinion or sent for peer-review.

Peer-review is the process by which other scientists judge your work anonymously. If they consider your work is scientifically sound and of interest to the community, they will recommend it be published. The paper is usually sent to 2 or 3 scientists and then the editor will make a decision based on the reviews.

This can be quite a difficult process because most of the reviews will come back with criticisms of the work. While it can be a little demoralising to receive such kind of feedback, take heart that incorporating such constructive criticism from outside the group into the body of the work invariable makes for a stronger study overall.

Usually a paper is submitted to the highest impact factor journal that seems plausible at first, and will be rejected with criticisms. These criticisms improve the paper, which will be submitted again, but this time to a lower impact journal and so on and so on. Overall these effects combat each other to create a natural bal-

> **Note**
>
> J. K. Rowling's 'Harry Potter' manuscript was rejected from the first 12 publishers to which she applied. Now it is a franchise worth billions! It can take a lot of time and patience to get published no matter how good your work.

ance where the work gets better even as it moves down the list of 'best' journals.

No matter what do not give up on a project. As long as your results are scientifically valid (which they will be for us to get to the stage of submitting for publication) then they will be accepted somewhere.

5.1.4 OPEN ACCESS

Most papers must be purchased to be read. If you have ever tried to access a paper outside of the university network you may have been asked to pay to download a pdf. This is why I insist all the information needs to be available in each paper; if someone pays for your article, they shouldn't have to pay for another article to understand what you did.

If a paper is made open-access, the authors pay so that everyone can read the paper for free. This massively increases the impact of the study because more people are likely to read it and cite it.

We should always try to make papers open access, but in reality it is too expensive for a group to pay for all of their papers to be published this way. I'll talk to you about this as necessary, but it's something you should be aware of.

5.2 PRESENTATIONS
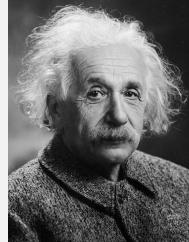
Presentations are usually made with powerpoint and composed of individual slides. Every slide should have a title, several slides can even have the same title but make sure there aren't any slides with no title. I find that text on a presentation is only useful if you refer to it specifically. I don't know anyone who can read and listen to two different sentences at the same time, and of course you want to make sure people are listening to you.

Most importantly relax. I've seen amazing projects be completely messed up by a speaker because they were afraid they would mess it up... isn't that silly? Even if somebody asks you the most difficult question you ever heard, you can respond that you'll look into it, or refer them to your supervisor (me).

I think most importantly, you should not need to memorise anything. The content of the presentation should be instructive for the audience but also be a prompt for you. If you are worried you will forget to say something, put that in the presentation specifically and this will remind you to talk about it. If it

> **Note**
>
> Sometimes students make things sound complicated to seem smart but I promise you this impresses no-one. Einstein was credited as saying 'If you can't explain it to a six year old, you don't understand it yourself'. Keep things simple!

doesn't matter whether you remember to say it or not, it doesn't need to be on the slide at all.

Some people disagree but I find animations are a great way to break a slide into sections. They also make sure the audience are focusing on the part you are talking about. If you have

3 images on a slide, the audience will look at all 3 of them as soon as they appear. If you use animations you can talk about the first, then make appear the next one, talk about that, then make the final one appear and conclude the slide. This becomes especially important at some of the larger conferences where they project on multiple screens, as you'll only be in a position to point at one version of the presentation.

I also think it's better if your talk is SHORTER than the allocated time slot rather than longer. Almost always the most important part of your talk is at the end, you will first introduce the topic, explain what you did and then explain the results. I have seen talks when someone spent 15 minutes introducing the topic and methods, but then was forced to stop before they could talk about their results. This makes all of the effort that went in to the presentation completely pointless.

5.3 JOB APPLICATIONS

Ultimately, no one can stay in a research group forever. Different job's in different fields will require their own evidence of experience and talent. I am happy to help you as much as I can to prepare these documents.
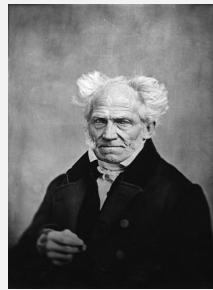
Every job you apply to will usually ask for an up-to-date curriculum vitae (CV) and cover letter, at the very least. A recent version of my own CV will be always available on-line for you to find. You can copy this directly but I advise against it, everyone's CV should be as unique as their life experience.

> **Note**
>
>
>
> The philosopher Arthur Schopenhauer said 'Every man mistakes the limit of his vision for the limits of the world'. There are more opportunities in society than you can possibly imagine! Spend some time to explore jobs and careers outside of academia.

While the same CV can usually be used for different job applications the cover letter should be specific for each application, to the point that the job title, company and location are mentioned explicitly in the letter. You should mention how the skills shown in your CV prove that you are an ideal candidate for the position and how you can bring something to the job that no-one else could.

Recommendation letters are also usually required for job applications. We should work together on a recommendation that you want me to provide for you. In it I can mention the specific things you have done that support your choice of future career, for example codes that you wrote if you wish to work in software development, or interpersonal interactions if you wish to work in teaching *etc*.

Because each person's requirements are different, I don't go any further in to details here but feel free to ask me any time.

6 SUMMARY

Hopefully this guide lays out the foundations for anyone wanting to work with us as a collaborator or a member. I tried to keep it as general as possible while still being informative.

Research can be daunting and difficult, especially because there's so much more to it than the basic science you learn at university. Don't worry if you saw something here that you don't use or didn't fully understand yet, sometimes the best way to learn about research is just to start doing it!

I will end the guide the same way I ended many of the sections: if you are ever unsure just ask me :)