



Burton Materials Data Lab 材料数据实验室

Group Guide 旅行指南



上海大学量子与分子结构国际研究中心
International Center of Quantum and Molecular Structures



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 working culture and group synergy to be one of 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 things, so 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 by me directly 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.²

Everyone should be constantly learning as they work. Try to always have a notebook to hand so that you can doodle ideas or quickly jot down paper details whenever they may come up. The physics of the methods,

Note

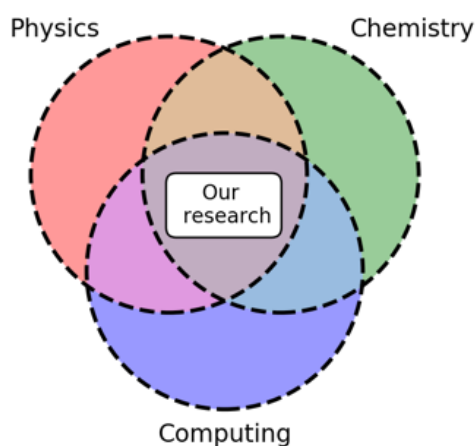


Margaret Thatcher had a PhD in chemistry and went on to become the first female prime-minister of the UK. The qualifications and skills you can obtain with us can be useful in almost any career path.

²V. Sekara, P. Deville, S. E. Ahnert, A.-L. Barabási, R. Sinatra, and S. Lehmann, "The chaperone effect in scientific publishing," PNAS, vol. 115, no. 50, pp. 12603–12607, 2018

the chemistry of the materials and the data science of the code packages all overlap in our area of research. No one person can understand all of these 3 areas, as they are individually developing rapidly in different directions, as shown in the Venn diagram below. 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 :)

Please try not to be wasteful in your printing, drafting and note-taking. I won't stop you from doing whatever you feel is necessary, so this is something you have to judge for yourself. Even running unnecessary calculations prevents other jobs from running, costs us money and uses energy so take care.



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 (Nobel prize in physics) famously said "if you think you understand quantum mechanics, you don't understand quantum mechanics." QM is just one of many areas we need to be familiar with, so don't feel bad if you don't understand everything.

3.2 YOURSELF

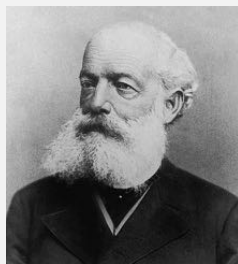
Research has to be challenging. If you think a project is easy that's because you are not pushing yourself. Science exists as a series of increasingly difficult models, from the cartoons you were taught as a child right up to the physical reality that is impossible to understand. Where you fall on this 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,^{3,4,5,6,7,8} 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,⁹ 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* WeChat for example, and we have no meetings scheduled then feel free to enjoy the beautiful scenery around Baoshan.

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

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!

³A. M. Isen, K. A. Daubman, and G. P. Nowicki, "Positive affect facilitates creative problem solving," *Journal of Personality and Social Psychology*, vol. 6, no. 52, pp. 1122–1131, 1987.

⁴F. G. Ashby, A. M. Isen, and A. U. Turken, "A neuropsychological theory of positive affect and its influence on cognition," *Psychological Review*, vol. 3, no. 106, pp. 529–550, 1999.

⁵B. L. Fredrickson, "The broaden-and-build theory of positive emotions," *Philos. Trans. R. Soc. Lond.*, vol. 359, no. 1449, pp. 1367–1378, 2004.

⁶A. K. Anderson, P. E. Wais, and J. D. E. Gabrieli, "Emotion enhances remembrance of neutral events past," *Proceedings of the National Academy of Sciences*, vol. 103, no. 5, pp. 1599–1604, 2006.

⁷G. Rowe, J. B. Hirsh, and A. K. Anderson, "Positive affect increases the breadth of attentional selection," *PNAS*, vol. 1, no. 104, pp. 383–388, 2007.

⁸A. J. Oswald, E. Proto, and D. Sgroi, "Happiness and productivity," *IZA Discussion*, no. 4645, p. 3, 2009.

⁹C. I. Seresinhe, T. Preis, G. MacKerron, and H. S. Moat, "Happiness is Greater in More Scenic Locations," *Scientific Reports*, vol. 9, no. 1, p. 4498, 2019.

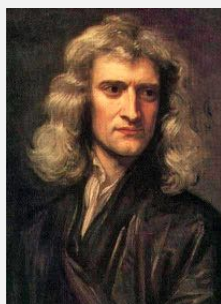
before you do, it can still be published and is valid as a body of work itself. If you are really having trouble please talk to me, but don't just try to switch projects because it's not as much fun as you first thought.

Manage your time and health properly. I guarantee you will be more productive working for 4 hours after an 8-hour sleep than you will working for the same 12 hours with no sleep, and other scientists see the same.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 (yes, I have had this happen). I once spent three days converting data tables and then on the third day thought up a line of code that could do the same job in less than 1 minute and contain no human errors. Having the patience, foresight and creativity that comes with being well rested can save a lot of time in the long-run.

There also is the danger of undoing good work that has already been done. I once 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 here. 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.^{13,14,15} I'm happy working 5 days of the week, but do you really need to work all 7? I won't stop you, but i encourage you to think more broadly about what 'work' means. If you go home to visit your parents and read papers on the way there, practice English via an app in your room, and then write a report on the train coming back, were you not working that day? As far as I am concerned I will not expect to see or hear from you on Saturday or Sunday. If you feel

¹⁰<https://www.sciencemag.org/careers/2019/04/academia-hard-work-expected-taking-break-effort-well-spent-too>

¹¹S. Guthrie *et al.* "Understanding mental health in the research environment: A Rapid Evidence Assessment", Santa Monica, Calif.: RAND Corporation, RR-2022-RS, 2017

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

¹³https://www.theguardian.com/world/2019/mar/12/string-of-british-firms-switch-over-to-four-day-working-week?CMP=Share_iOSApp_Other

¹⁴<https://www.nytimes.com/2018/07/19/world/asia/four-day-workweek-new-zealand.html>

¹⁵https://www.huffingtonpost.com/entry/four-day-working-week-overwork-life-balance_us_5c360351e4b0f5aba7da3d5a

you must work that's fine, but otherwise i hope you can enjoy these days in whatever way suits you.

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.¹⁶ 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, still win the title of most innovative company.¹⁷

If you are ever sick, please do NOT come to the office. I know some people think that this is a great 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 some work while outside of the office. We can arrange Skype meetings or alternatives so that progress in your research can still be made. However, overall you will be most productive at the office and, if you are able to do so, please try to be around campus between 9am-5pm.

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 talk

to me, I will not consider it a demerit. I already said i won't expect to see you outside of a 9am-5pm, 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

¹⁶<https://mashable.com/2018/05/11/google-20-percent-rule/#UuoJ09zf5kqU>

¹⁷<https://which-50.com/google-not-apple-named-bcgs-most-innovative-company-in-2019/>

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 lost small 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. My first week in Shanghai I was asked if I would like to buy some beard (I can grow my own face hair thank you!) but they were really asking if i would like to buy some BREAD. I've also been asked if i was hungry for a snake (SNACK), if i went there by sheep (SHIP) or if i liked to eat stick (STEAK). This is certainly 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'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 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 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? *etc.*

It's an unfortunate truth that I will need more help from you than Chinese 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 dead-

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.

lines. 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.

Note



Cecilia Payne was the first person to discover that stars are made of H_2 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."

I know some of concepts I discuss are not standard ideas for a Chinese research group and a lot of them can be interpreted as sheer laziness from an outside perspective. If any member of staff or other students give you problems because you don't spend 12 hours

each day in the office, tell them to bring their issue to me and not complain to you. As long as I'm happy with your output and we're meeting the requirements of the university, it doesn't matter what others think.

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.