

## Course Information Sheet for entry in 2021-22: DPhil in Computational Discovery



This innovative course has been developed in close partnership between Oxford University and IBM Research. Each research project has been co-developed by Oxford academics working with IBM scientists. Students will have a named IBM supervisor/s and many opportunities for collaboration with IBM throughout the studentship.

The scientific focus of the programme is at the interface between Physical and Life Sciences. By bringing together advances in data and computing science with large complex sets of experimental data, more realistic and predictive computational models can be developed. These new tools and methodologies for computational discovery can drive advances in our understanding of fundamental cellular biology and drug discovery. Projects will span the emerging fields of Advanced Molecular Simulations, Machine Learning, and Quantum Computing while addressing both fundamental questions in each of these fields as well as at their interfaces.

Students will benefit from the interdisciplinary nature of the course cohort as well as the close interactions with IBM Scientists. After a very short induction period of one or two weeks, during which some basic training is provided, you will start a research project in your academic supervisor's laboratory.

Most laboratories have weekly meetings where members present and discuss their research results with other members of the laboratory. You will also regularly present your work in progress seminars, which are attended by other research groups working in related areas.

Whilst working on your research project you will participate in a comprehensive, flexible skills training programme which includes a range of workshops and seminars in transferable skills, generic research skills and specific research techniques. There are also numerous seminars and lectures by local and visiting scientists and you are provided with many opportunities to meet leading scientists.

### Projects and supervisors available for entry in 2021-22

Projects will be available across three related themes. Topics will include both fundamental and applied in each field. Particular focus will be given to interdisciplinary research at the interface of the three fields.

#### Theme One: Advanced Molecular Simulations

1. Improved physical models of bio-materials
2. Protein-membrane interactions
3. Using molecular dynamic simulations to advance drug discovery or medicinal chemistry
4. Combining computational and structural biology approaches to molecular discovery

Please contact the Theme Lead Phil Biggin if you have any questions about these projects.

#### Theme Two: Artificial Intelligence and Machine Learning

1. Fundamental methodologies for ML
2. Neuroscience inspired AI
3. Applications of ML in molecular discovery

Please contact the Theme Lead Mihai Cucuringu if you have any questions about these projects.

#### Theme Three: Quantum Computing

1. Algorithm development
2. Applications in chemistry and molecular simulations
3. Interface of Quantum and Classical computing

Please contact the Theme Lead Dieter Jaksch if you have any questions about these projects.

### Supervision

The allocation of graduate supervision is the responsibility of the Medical Sciences Graduate School and it is not always possible to accommodate the preferences of incoming graduate students to work with a particular member of staff. Under exceptional circumstances a supervisor may be found outside the department leading the course.

Your supervisor may appoint a senior member of the laboratory as your day-to-day supervisor. Further support is available from your college advisor.

### Assessment

There are a number of key stages in the research programme. Within a month of starting, you will meet with your academic and IBM supervisors to finalise your project and agree on an initial programme of research. Within the first three months, you will complete an analysis of your training needs with your academic supervisor.

Students begin the DPhil in Computational Discovery programme as a probationary research student (PRS). Before the end of their fourth term students are required to apply for Transfer to DPhil Status.

A successful transfer of status from PRS to DPhil status will require the submission of a transfer report. Students who are successful at transfer will also be expected to apply for and gain confirmation of DPhil status to show that their work continues to be on track. This will need to be done within nine terms of admission.

Both milestones normally involve an interview with two assessors (other than your supervisor) and therefore provide important experience for the final oral examination.

You will be expected to submit an original thesis of up to 50,000 words after three or, at most, four years from the date of admission. To be successfully awarded a DPhil you will need to defend your thesis orally (viva voce) in front of two appointed examiners.

The frequency of meetings with supervisors will depend on which department your DPhil is based. Commonly, within those departments based with the Medical Science Division, once a fortnight is typical.

### Changes to courses

The University will seek to deliver this course in accordance with the description set out above. However, there may be situations in which it is desirable or necessary for the University to make changes in course provision, either before or after registration. These may include significant changes made necessary by a pandemic (including Covid-19), epidemic or local health emergency. For further information, please see the University's Terms and Conditions (<http://www.graduate.ox.ac.uk/terms>) and our page on changes to courses (<http://www.graduate.ox.ac.uk/coursechanges>).

### Expected length of course

	Full Time Only
Expected length	3 to 4 years

## Costs

### Annual fees for entry in 2021-22

Fee status	Annual Course fees
Home (UK, Republic of Ireland, Channel Islands & Isle of Man)	£8,290
Overseas (including EU)	£27,460

Course fees are payable each year, for the duration of your fee liability (your fee liability is the length of time for which you are required to pay course fees). For courses lasting longer than one year, please be aware that fees will usually increase annually. Information about how much fees and other costs may increase is set out in the University's Terms and Conditions.

Course fees cover your teaching as well as other academic services and facilities provided to support your studies. Unless specified in the additional cost information (below), course fees do not cover your accommodation, residential costs or other living costs. They also don't cover any additional costs and charges that are outlined in the additional cost information.

Graduate students who have reached the end of their standard period of fee liability may be required to pay a termly University and/or a college continuation charge.

The University continuation charge, per term for entry in 2021-22 is £528, please be aware that this will increase annually. For part-time students, the termly charge will be half of the termly rate payable by full-time students.

If a college continuation charge applies (not applicable for non-matriculated courses) it is likely to be in the region of £100 to £400 per term. Please contact your college for more details.

### Additional cost information

There are no compulsory elements of this course that entail additional costs beyond fees (or, after fee liability ends, continuation charges) and living costs. However, please note that, depending on your choice of research topic and the research required to complete it, you may incur additional expenses, such as travel expenses, research expenses, and field trips. You will need to meet these additional costs, although you may be able to apply for small grants from your department and/or college to help you cover some of these expenses.

## Living costs

In addition to your course fees, you will need to ensure that you have adequate funds to support your living costs for the duration of your course.

The likely living costs for 2021-22 are published below. These costs are based on a single, full-time graduate student, with no dependants, living in Oxford. We provide the cost per month so you can multiply up by the number of months you expect to live in Oxford.

Likely living costs for 2021-22

	Likely living costs for 1 month		Likely living costs for 9 months		Likely living costs for 12 months	
	Lower range	Upper range	Lower range	Upper range	Lower range	Upper range
<b>Food</b>	£280	£400	£2,520	£3,600	£3,360	£4,800
<b>Accommodation</b>	£655	£790	£5,895	£7,110	£7,860	£9,480
<b>Personal items</b>	£130	£250	£1,170	£2,250	£1,560	£3,000
<b>Social activities</b>	£45	£115	£405	£1,035	£540	£1,380
<b>Study costs</b>	£45	£100	£405	£900	£540	£1,200
<b>Other</b>	£20	£55	£180	£495	£240	£660
<b>Total</b>	£1,175	£1,710	£10,575	£15,390	£14,100	£20,520

When planning your finances for any future years of study at Oxford beyond 2021-22, you should allow for an estimated increase in living expenses of 3% each year.

More information about how these figures have been calculated is available at [www.graduate.ox.ac.uk/livingcosts](http://www.graduate.ox.ac.uk/livingcosts).

## Document accessibility

If you require an accessible version of the document please contact Graduate Admissions and Recruitment by email ([graduate.admissions@admin.ox.ac.uk](mailto:graduate.admissions@admin.ox.ac.uk)) or via the online form (<http://www.graduate.ox.ac.uk/ask>).