



## DEPARTMENT OF CHEMISTRY

### Summary

<b>Job title</b>	Postdoctoral Research Associate in Computational Materials Chemistry
<b>Division</b>	Mathematical, Physical and Life Sciences
<b>Department</b>	Department of Chemistry
<b>Location</b>	Inorganic Chemistry Laboratory, South Parks Road, Oxford OX1 3QR
<b>Grade and salary</b>	Grade 7: £36,024 - £44,263 per annum
<b>Hours</b>	Full time
<b>Contract type</b>	Fixed-term for a period of up to 24 months
<b>Reporting to</b>	Professor Volker Deringer
<b>Vacancy reference</b>	174819
<b>Additional information</b>	The post is available as soon as possible

<b>Research topic</b>	Amorphous Materials by Design through Atomistic Understanding
<b>Principal Investigator / supervisor</b>	Professor Volker Deringer
<b>Project web site</b>	<a href="https://www.chem.ox.ac.uk/people/volker-deringer">https://www.chem.ox.ac.uk/people/volker-deringer</a>
<b>Funding partner</b>	The funds supporting this research project are provided by UK Research and Innovation



## The role

Applications are invited for a Postdoctoral Research Associate to work in the Deringer research group within the Inorganic Chemistry Laboratory at Oxford. Our research is in computational materials chemistry, with a particular interest in structures and properties of amorphous materials. We have been awarded a prestigious UKRI Frontier Research grant which will provide the funding for this post. The post is available for a period of up to 24 months.

The project involves the development and application of machine-learning based interatomic potential models. The postholder will develop protocols and workflows for fitting ML potentials and apply them to a range of research questions in the area of amorphous functional materials.

The group's research vision is to understand, and ultimately to control, materials structure based on accurate atomic-scale simulations. We have a strong track record in using ML-driven modelling to study the structure of inorganic materials.

## Responsibilities

1. Manage own academic research and administrative activities. This involves small scale project management, to co-ordinate multiple aspects of work to meet deadlines
2. Adapt existing and develop new scientific techniques and computational protocols
3. Use specialist scientific equipment including Linux workstations and high-performance computing clusters
4. Test hypotheses and analyse scientific data from a variety of sources, reviewing and refining working hypotheses as appropriate
5. Contribute ideas for new research projects and directions, develop ideas for generating research income, contribute to bids for funding and computing resources when asked, and present detailed research proposals to senior researchers
6. Undertake comprehensive and systematic literature reviews
7. Write up the results of the research for publication in peer-reviewed journals, collaborate in the preparation of scientific reports and journal articles, and occasionally present papers and posters
8. Represent the research group at external meetings / seminars, either with other members of the group or alone
9. PDRAs may be required to teach; this may include lecturing, small-group teaching, and tutoring of undergraduates and graduate students.

## Selection criteria

### Essential selection criteria

1. Hold a PhD in Chemistry or a related area (or be close to completion), prior to taking up the appointment.
2. Be able to demonstrate experience and expertise in the parameterisation, validation, and application of machine-learning-based interatomic potential models for inorganic materials.

3. Have expertise with large-scale molecular-dynamics simulations of inorganic materials using high-performance computing facilities, including use of the LAMMPS software, and demonstrated competence in managing computational resources.
4. Be able to demonstrate competence and success in the thesis research area (and postdoctoral work if appropriate), e.g. as judged by publications in high quality peer reviewed journals and / or preprints. Evidence will be sought of a deep understanding of the applicant's previous fields of research and evidence of independent intellectual and practical contributions to previous research projects, as indicators that such attributes can be brought to bear on the present project.
5. Be viewed as a motivated, enthusiastic, organised self-starter; one who can work with a minimum of supervision but at the same time extract the benefits of an excellent research environment.
6. Have an excellent general knowledge of related areas through reading of the literature, online database searching, and attendance at seminars and conferences.
7. Be willing to learn new techniques and apply them in an interdisciplinary research environment. Be willing to participate in group journal clubs and workshops as a means to continuously improve technical and theoretical knowledge.
8. Communicate well in English in writing and in oral and visual presentations, and be able to create high-quality scientific illustrations for publications and other purposes with minimal supervision.
9. Be able to keep detailed records of computational work and report on progress at regular intervals. Demonstrate ability and willingness to maintain best practices in data management, including the use of repositories for publishing research data.
10. Show an ability to work supportively in a computational chemistry research group, and to supervise and educate junior co-workers and take part in joint projects through co-operation and the exchange of information, data, and code. Be willing to play a role in keeping the laboratory running by assuming a share of group responsibilities.

#### Desirable selection criteria

1. Have expertise in the atomistic modelling of amorphous materials and the computational study of their properties.

### Pre-employment screening

#### Standard checks

If you are offered the post, the offer will be subject to standard pre-employment checks. You will be asked to provide: proof of your right-to-work in the UK; proof of your identity; and (if we haven't done so already) we will contact the referees you have nominated. You will also be asked to complete a health declaration so that you can tell us about any health conditions or disabilities for which you may need us to make appropriate adjustments.

Please read the candidate notes on the University's pre-employment screening procedures at:

<https://www.jobs.ox.ac.uk/pre-employment-checks>

### About the University of Oxford

Welcome to the University of Oxford. We aim to lead the world in research and education for the benefit of society both in the UK and globally. Oxford's researchers engage with academic, commercial and cultural partners across the world to stimulate high-quality research and enable innovation through a broad range of social, policy and economic impacts.

We believe our strengths lie both in empowering individuals and teams to address fundamental questions of global significance, while providing all our staff with a welcoming and inclusive workplace that enables everyone to

develop and do their best work. Recognising that diversity is our strength, vital for innovation and creativity, we aspire to build a truly diverse community which values and respects every individual's unique contribution.

While we have long traditions of scholarship, we are also forward-looking, creative and cutting-edge. Oxford is one of Europe's most entrepreneurial universities and we rank first in the UK for university spin-outs, and in recent years we have spun out 15-20 new companies every year. We are also recognised as leaders in support for social enterprise.

Join us and you will find a unique, democratic and international community, a great range of staff benefits and access to a vibrant array of cultural activities in the beautiful city of Oxford.

For more information, please visit [www.ox.ac.uk/about/organisation](http://www.ox.ac.uk/about/organisation).

## Department Of Chemistry

The mission of Oxford Chemistry is to advance the global understanding of chemistry and to use that knowledge to address major challenges for society. Oxford Chemistry maintains world-class strengths in fundamental research, including the training of outstanding young scientists, whilst being an outward-looking department engaging with other disciplines, industry, public services, government and the general public. We are a large department within the University's Mathematical, Physical and Life Sciences Division with over 70 research groups and 900 researchers including 400 graduate research students. Our MChem degree takes 180 students a year and features the distinctive tutorials of Oxford, an innovative three-year programme of practical teaching within our state-of-the-art teaching laboratory, and a 4th year focused on research based within one of our research groups.

Research in Oxford Chemistry focuses on fundamental science aimed at making significant and sustained long-term impact. We provide an environment that enables research by hiring, developing, and supporting talented researchers, many recognised as international leaders, across the spectrum of the chemical sciences. Our students and staff work in excellent research facilities to deliver field-leading research that crosses traditional boundaries and engages strongly with other disciplines, both within Oxford and across a range of external sectors.

The impact of our research in the wider economy and society is manifest in our many industrial and clinical collaborations and successful start-ups. Our eight research themes and business engagements showcase the breadth and depth of our research across the chemical sciences.

We are committed to providing an inclusive and supportive work and study environment for all our staff and students based on core values of respect, equality and collaboration. We have held an Athena SWAN silver award since 2015 reflecting our commitment to improving gender equality within our discipline.

Oxford Chemistry is accommodated within five buildings in the University's science area, including a modern RIBA award-winning dedicated research facility and a state-of-the-art practical teaching laboratory. Researchers are supported by a research infrastructure within Chemistry that includes NMR, Mass Spectrometry, Crystallography, Surface Analysis, Inorganic Materials Characterisation, Advanced Electron Spin Resonance and high-performance computing facilities as well as access to facilities across the wider University and at national research facilities including the Rosalind Franklin Institute and Diamond Light Source.

To support the Teaching and Research in the Department, there are a number of administrative functions including Finance, Human Resources, Facilities, Information Technology, Student Administration, Health and Safety, Communications and Alumni Relations.

Find out more about the Department, our work and our people at [chem.ox.ac.uk](http://chem.ox.ac.uk)

## Equality, Diversity and Inclusion in Oxford Chemistry

We are committed to promoting an inclusive and diverse community of students and staff based on core values of respect, equality and collaboration. The Department has an active Equality, Diversity and Inclusion (EDI) committee and since 2015 we have held an Athena SWAN silver award in recognition of our efforts to introduce organisational and cultural practices which promote gender equality and create a better working environment for all. We promote family-friendly policies and support flexible working arrangements where possible. For more information about the University's family friendly benefits, please also see <https://hr.admin.ox.ac.uk/information-for-parents-and-carers>

## Mathematical, Physical and Life Sciences Division

The academic administration of the University is conducted through four divisions (Humanities, Social Sciences, Mathematical, Physical and Life Sciences, and Medical Sciences). The Mathematical, Physical and Life Sciences Division consists of ten constituent departments: The Department of Chemistry, the Department of Computer Science, the Department of Earth Sciences, the Department of Engineering Science, the Department of Materials, Mathematical Institute, the Department of Physics, Department of Plant Sciences, Department of Zoology and the Department of Statistics. The division provides a framework for interdisciplinary teaching and research. There are also links with the Medical Sciences Division.

The disciplines within the MPLS Division regularly appear at the highest levels in rankings, including the Times Higher Education and QS world rankings. Nationally, the quality of the Division's research outputs and environment, and the resulting impact, was recognised through strong performances in the UK Research Excellence Framework in both 2014 and 2021.

For more information please visit: <http://www.mpls.ox.ac.uk/>

## How to apply

Applications are made through our online recruitment portal. Information about how to apply is available on our Jobs website <https://www.jobs.ox.ac.uk/how-to-apply>.

Your application will be judged solely on the basis of how you demonstrate that you meet the selection criteria stated in the job description.

As part of your application you will be asked to provide details of **two referees and indicate whether we can contact them now**.

You will be asked to upload a CV and a supporting statement. The supporting statement must explain how you meet each of the selection criteria for the post using examples of your skills and experience. This may include experience gained in employment, education, or during career breaks (such as time out to care for dependants)

Please upload all documents **as PDF files** with your name and the document type in the filename.

All applications must be received by **midday** UK time on the closing date stated in the online advertisement.

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## Information for priority candidates

A priority candidate is a University employee who is seeking redeployment because they have been advised that they are at risk of redundancy, or on grounds of ill-health/disability. Priority candidates are issued with a redeployment letter by their employing department(s).

If you are a priority candidate, please ensure that you attach your redeployment letter to your application (or email it to the contact address on the advert if the application form used for the vacancy does not allow attachments).

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## If you need help

Application FAQs, including technical troubleshooting advice is available at:

<https://staff.web.ox.ac.uk/recruitment-support-faqs>

Non-technical questions about this job should be addressed to the recruiting department directly

[recruitment@chem.ox.ac.uk](mailto:recruitment@chem.ox.ac.uk)

To return to the online application at any stage, please go to: [www.recruit.ox.ac.uk](http://www.recruit.ox.ac.uk).

Please note that you will receive an automated email from our online recruitment portal to confirm receipt of your application. **Please check your spam/junk mail** if you do not receive this email.

## Important information for candidates

### Data Privacy

Please note that any personal data submitted to the University as part of the job application process will be processed in accordance with the GDPR and related UK data protection legislation. For further information, please see the University's Privacy Notice for Job Applicants at: <https://compliance.admin.ox.ac.uk/job-applicant-privacy-policy>. The University's Policy on Data Protection is available at: <https://compliance.admin.ox.ac.uk/data-protection-policy>.

### The University's policy on retirement

The University operates an Employer Justified Retirement Age (EJRA) for very senior research posts at **grade RSIV/D35 and clinical equivalents E62 and E82** of 30 September before the 70<sup>th</sup> birthday. The justification for this is explained at: <https://hr.admin.ox.ac.uk/the-ejra>.

For **existing** employees on these grades, any employment beyond the retirement age is subject to approval through the procedures: <https://hr.admin.ox.ac.uk/the-ejra>.

There is no normal or fixed age at which staff in posts at other grades have to retire. Staff at these grades may elect to retire in accordance with the rules of the applicable pension scheme, as may be amended from time to time.

### Equality of opportunity

Entry into employment with the University and progression within employment will be determined only by personal merit and the application of criteria which are related to the duties of each particular post and the relevant salary structure. In all cases, ability to perform the job will be the primary consideration. No applicant or member of staff shall be discriminated against because of age, disability, gender reassignment, marriage or civil partnership, pregnancy or maternity, race, religion or belief, sex, or sexual orientation.

## Benefits of working at the University

### Employee benefits

University employees enjoy 38 days' paid holiday, generous pension schemes, travel discounts, and a variety of professional development opportunities. Our range of other employee benefits and discounts also includes free entry to the Botanic Gardens and University colleges, and discounts at University museums. See <https://hr.admin.ox.ac.uk/staff-benefits>

### University Club and sports facilities

Membership of the University Club is free for all University staff. The University Club offers social, sporting, and hospitality facilities. Staff can also use the University Sports Centre on Iffley Road at discounted rates, including a fitness centre, powerlifting room, and swimming pool. See [www.club.ox.ac.uk](http://www.club.ox.ac.uk) and <https://www.sport.ox.ac.uk/>.

### Information for staff new to Oxford

If you are relocating to Oxfordshire from overseas or elsewhere in the UK, the University's Welcome Service website includes practical information about settling in the area, including advice on relocation, accommodation, and local schools. See <https://welcome.ox.ac.uk/>

There is also a visa loan scheme to cover the costs of UK visa applications for staff and their dependants. See <https://staffimmigration.admin.ox.ac.uk/visa-loan-scheme>

### Family-friendly benefits

With one of the most generous family leave schemes in the Higher Education sector, and a range of flexible working options, Oxford aims to be a family-friendly employer. We also subscribe to the Work+Family Space, a service that provides practical advice and support for employees who have caring responsibilities. The service offers a free telephone advice line, and the ability to book emergency back-up care for children, adult dependents and elderly relatives. See <https://hr.admin.ox.ac.uk/my-family-care>

The University has excellent childcare services, including five University nurseries as well as University-supported places at many other private nurseries.

For full details, including how to apply and the costs, see <https://childcare.admin.ox.ac.uk/>

### Disabled staff

We are committed to supporting members of staff with disabilities or long-term health conditions. For further details, including information about how to make contact, in confidence, with the University's Staff Disability Advisor, see <https://edu.admin.ox.ac.uk/disability-support>

### Staff networks

The University has a number of staff networks including the Oxford Research Staff Society, BME staff network, LGBT+ staff network and a disabled staff network. You can find more information at <https://edu.admin.ox.ac.uk/networks>

### The University of Oxford Newcomers' Club

The University of Oxford Newcomers' Club is an organisation run by volunteers that aims to assist the partners of new staff settle into Oxford, and provides them with an opportunity to meet people and make connections in the local area. See [www.newcomers.ox.ac.uk](http://www.newcomers.ox.ac.uk).

### Oxford Research Staff Society (OxRSS)

A society run by and for Oxford University research staff. It offers researchers a range of social and professional networking opportunities. Membership is free, and all researchers employed by Oxford University are welcome to join. Subscribe at [researchstaff-subscribe@maillist.ox.ac.uk](mailto:researchstaff-subscribe@maillist.ox.ac.uk) to join the mailing list to find out about upcoming events and other information for researchers, or contact the committee on [committee@oxrss.ox.ac.uk](mailto:committee@oxrss.ox.ac.uk). For more information, see [www.ox.ac.uk/oxrss](http://www.ox.ac.uk/oxrss), Twitter @ResStaffOxford, and Facebook [www.facebook.com/oxrss](http://www.facebook.com/oxrss).