

Salary: £39,748- £44,166 per annum (dependent on skills and experience). Specialist allowance of up to £4k per annum depending on experience and access to STFC UK VISA support. Support (up to £8k) for UK VISA (healthcare) costs through the relevant skilled worker routes.

Hours: Full time

Contract Type: Open Ended.

Location: Science and Technology Facilities Council, Rutherford Appleton Laboratory Harwell, Oxfordshire OR Science and Technology Facilities Council, Daresbury Laboratory, Warrington

We are the Scientific Computing Department (SCD), part of the UK National Laboratories at UKRI STFC, based at the Daresbury Laboratory (Warrington) and the Rutherford Appleton Laboratory (Oxfordshire). We perform research as well as developing and providing computing services that enable more and better research across the UK and beyond. Our expertise and capability span across the full range of the computing stack – from large-scale computing facilities, computing data services and infrastructure to numerical analysis, software engineering, AI, and computational science, theory development included.

The Theoretical and Computational Physics Group (TPCG [1]) is part of SCD. We are an international, family friendly, diverse group who have played a central role in many ground-breaking UK code development projects including CASTEP, CRYSTAL, ONETEP, Wannier90, and QUESTAAL. We are active in a large number of diverse scientific projects and collaborations with the UK and overseas, and also work in direct collaboration with the STFC large experimental Facilities (Diamond Light Source, ISIS neutron and muon source, the Central Laser Facility).

We are currently looking for three Computational Scientists to join our group. The successful applicants will join a rapidly growing initiative aimed at transforming research performed at large experimental Facilities (synchrotrons, neutron and muon sources, laser-based facilities etc) through a multi-disciplinary approach to data processing, computer simulation and data analytics. This initiative will provide computing hardware, build software and provide computational and data analytics expertise that will spark a paradigm shift in the capability of scientists to design, analyse and interpret experiments.

About the roles:

We are open to consider applicants across a broad range of interests at the confluence between first principles methods and experimental materials science. The ultimate aim of your work will be to advance the science performed at experimental Facilities by improving either data interpretation, experiment design, or facility operation.

To this aim, you will undertake research to develop computational tools based on first principles theories and implement these in software within well-established computational and experimental user communities. You will also use these computational tools to collaborate with Facilities scientists and users on specific application projects.

You will become involved with a number of different codes, both at the development and application levels, and demonstrate the ability to lead and develop new scientific projects effectively, collaborating with both the first principles materials simulation community and STFC experimental Facilities.

Depending on your inclinations and skills, you will be also offered the possibility to contribute, via development and application of suitable first principles materials simulation methods and related workflows to the continuous development of large-scale facility technologies, starting from, but not limited to, the design, screening and development of innovative solutions for underpinning components or elements (beamline materials included) of the Facility experiment.

Additional development of synergies and follow up opportunities with existing EPSRC-funded materials physics/chemistry research (e.g. [2-4]) and community-focused software development initiatives (e.g. [5-9]) active at the TPCG will not only be possible but strongly encouraged.

1. <https://www.scd.stfc.ac.uk/Pages/Theoretical-and-Computational-Physics-Group.aspx>
2. [EP/S031081/1](#). 3. [EP/V048279/1](#). 4. [EP/T027916/1](#)
5. [EP/T026375/1](#). 6. [EP/X035891/1](#). 7. [EP/W030438/1](#). 8. [EP/W029480/1](#). 9. [EP/W026775/1](#)

We are especially interested in applications from candidates with track record and ambitions in one or more of the following specific areas (not necessarily all of them from the same candidate):

- Theoretical and/or methodological and/or workflow developments to interpret and exploit the results of experimental measurements at large experimental Facilities
- Software optimisation and parallelization
- Engage at the scientific level with relevant communities, through networking, as well as organizing workshops and delivering hands-on courses and training as required
- Application and/or extension of first principles methods and software to materials of scientific or technological interest
- Drafting of scientific papers and/or Facility technical reports demonstrating the new functionalities developed and implemented in (Facility) accessible software
- Active role in the drafting of scientific proposals to leverage external or STFC-internal resources

About you

These are highly collaborative roles, and you will work closely with a variety of people, as such the ability to interact and communicate well with others is a must. You must have the ability to develop good working relationships and be eager to develop skills in the interaction with experimental scientists.

Essential Criteria:

- PhD in Computational Physics, Chemistry, Materials Science or related area
- Expertise in condensed matter or computational materials physics or chemical physics
- Well versed in the development and application of Density Functional Theory (DFT) or beyond DFT approaches with a special focus on interpretation of large-scale Facility experiments
- Experience in the development and documentation of first principles materials simulation software
- Experience, commensurate to the career stage and previous working experience, in peer-reviewed dissemination of computational science research
- Significant experience in using High Performance Computing resources
- Extensive experience with software development in compiled languages e.g. FORTRAN and/or C++
- Excellent communication skills in spoken and written English
- Proven skills in taking (co-)responsibility for the management and time-effective delivery of scientific and/or software tasks of medium complexity
- Given that the large UK Facilities are based at the Rutherford Appleton Laboratory, availability to travel and regular visits at the Rutherford Appleton Laboratory will be expected for the successful applicants who may choose Daresbury Laboratory as their main work site.
- Regardless of the location, you will be expected to pursue and promote scientific interactions across the group and its varied activities.

Desirable Criteria:

- Experience with team-working and, ideally, co-development of scientific software
- Experience (or keen to develop experience) in effective collaboration with scientists of experimental background and/or facility beam-scientists
- Experience with as many as possible between a) DFT and/or beyond-DFT electronic structure methods, b) simulation of correlated-electron systems, c) simulation of ground-state and/or excited-state electronic and/or nuclear response functions in materials, d) theory and simulation of superconductivity and/or electron-phonon coupling, e) Quantum Monte Carlo, f) advanced structure and dynamics sampling methods, g) non-linear optical spectroscopies, h) simulation of coatings and/or solid/solid (solid/liquid) interfaces, i) thermal DFT or alternative approaches for warm dense matter
- Experience with distributed (MPI) and/or hybrid (MPI-OMP, CPU-GPU) parallel programming

- Experience with software development in interpreted languages e.g. PYTHON
- Excellent track-record, commensurate to the career stage and previous working experience, in peer-reviewed dissemination of scientific work
- Track-record, commensurate to the career stage and previous working experience, in leverage of external funding, HPC resources included

How to apply

Please apply for this role via the UKRI careers portal by following this link:

https://careersportal.taleo.net/careersection/ukri_int/jobdetail.ftl?job=2200014B&tz=GMT+00:00&tzname=Europe/London

When applying for this role please include in your cover letter (no word limit in principle) also an additional scientific statement of no more than 1300 words highlighting your ambitions in computational physics over the next five years with the TCGP & STFC. Applicants without the statement will not be considered

Please include (in either your cover letter or your CV) also the details of at least 2 referees (who will not be contacted without your permission)

If you have an informal enquiries about this position, please contact the TCGP group leader, Dr Gilberto Teobaldi (gilberto.teobaldi@stfc.ac.uk)

Application deadline: Sunday 26 February 2023

Benefits

- 30 days leave plus public holidays (pro rata)
- Christmas shutdown
- An onsite subsidised nursery
- An outstanding career average revalued earnings pension scheme
- Flexible working hours
- Employee shopping/travel discounts
- A salary sacrifice cycle to work scheme

We are committed to sustaining a diverse and inclusive workforce. We are invested in creating an environment that is welcoming and supportive of all and we strongly encourage applications from under-represented groups.