A Postdoctoral Research Fellow is available in the School of Chemistry at the University of Southampton working in the research group of Professor Graeme Day, as part of a team developing methods and applications of crystal structure modelling.

Apply here: https://jobs.soton.ac.uk/Vacancy.aspx?ref=911717EB

The research project is in collaboration with Professor Andrew Cooper (University of Liverpool) and forms part of the Leverhulme Centre for Functional Materials Design, recently funded by the Leverhulme Trust. You will apply and develop the research group's computational methodologies for crystal structure and property prediction to guide the experimental discovery of novel functional materials. The work will build on our work recently published in *Nature* (2017) <u>543</u>, 657-664, *Nature Chemistry* (2017), <u>9</u>, 17-25, *ACS Central Science* (2017) <u>3</u>, 734-742 and the *Journal of Materials Chemistry C* (2017) <u>5</u>, 7574-7584.



organic semiconductor screening: J. Mat. Chem. C (2017), 5, 7574-7584

Applications are invited from candidates having, or about to obtain a *PhD in chemistry, physics, or a related area, with a solid grounding in computational chemistry. You are expected to have an excellent work ethic and commitment to achieve the project aims, as well as excellent organisational skills in order to manage the research project on a day to day basis. You will also have opportunities to develop your supervision, writing, and communication skills. Duties will also include assisting in the training and supervision of PhD and undergraduate project students.

*Applications will be considered from candidates who are working towards or nearing completion of a relevant PhD qualification. The title of Research Fellow will be applied upon completion of PhD. Prior to the qualification being awarded the title of Senior Research Assistant will be given.

You will be based in the computational systems chemistry sector in the School of Chemistry at the University of Southampton. Chemistry at Southampton has a national and international reputation for excellence. The university hosts excellent high performance computing facilities (https://www.southampton.ac.uk/isolutions/staff/iridis.page) and the project will also make use of national computing resources.

The position is available for 36 months on a full time basis. The starting salary will be in the range \pm 29,301 - \pm 32,958 per annum. Candidates must be able to demonstrate their eligibility to work in the UK in accordance with the Immigration, Asylum and Nationality Act 2006. Where relevant this may include entry clearance or continued leave to remain under the Points Based Immigration Scheme.

At the University of Southampton, we value diversity and equality.

For further information about the Day research group and their research, see:

http://www.crystalstructureprediction.net

For information about Chemistry at Southampton see: <u>http://www.southampton.ac.uk/chemistry</u>

For informal enquiries, please contact Professor Graeme Day, g.m.day@soton.ac.uk

About the Leverhulme Centre for Functional Materials Design.

https://www.liverpool.ac.uk/leverhulme-research-centre/

The Centre is one of only 4 such centres funded in the UK and brings together chemical knowledge with state-of-the-art computer science and automated technologies to develop a new approach to revolutionise the design of functional materials at the atomic scale.

The centre is led by the University of Liverpool and involves a world leading multidisciplinary team including partners from the University of Southampton, Imperial College, the Hartree Centre, Diamond Light Source, the Cambridge Crystallographic Data Centre, King Abdullah University of Science and Technology, and the Max Planck Institute for Microstructure Physics, This team will help bridge the current 'design gap' by fusing leading-edge synthesis concepts from the physical sciences with ideas from the forefront of computer science, alongside experts in robotics, engineering, management and social science.

The vision is to create a disruptive new design capability by fusing four interacting themes in computational and experimental design, intelligent automation, and knowledge exploitation. This will enable dynamic cross-boundary working to arrange atoms and molecules with unprecedented control to create function. In its early years, the Centre will build dialogue and understanding between the disciplines, for example to develop state-of-the-art computer science algorithms for chemical structure prediction problems. Management research will inform interdisciplinary working practice in the Centre, which will include training in the socioeconomic global context for materials discovery. As the Centre evolves, we will exemplify this growing capability by tackling currently intractable design problems to discover exciting new functional materials, such as synthetic enzymes, superconductors, or materials for energy storage / generation; further application-specific development of these systems, beyond the discovery and understanding stage, will exit the core Centre funding, to retain our capability focus.