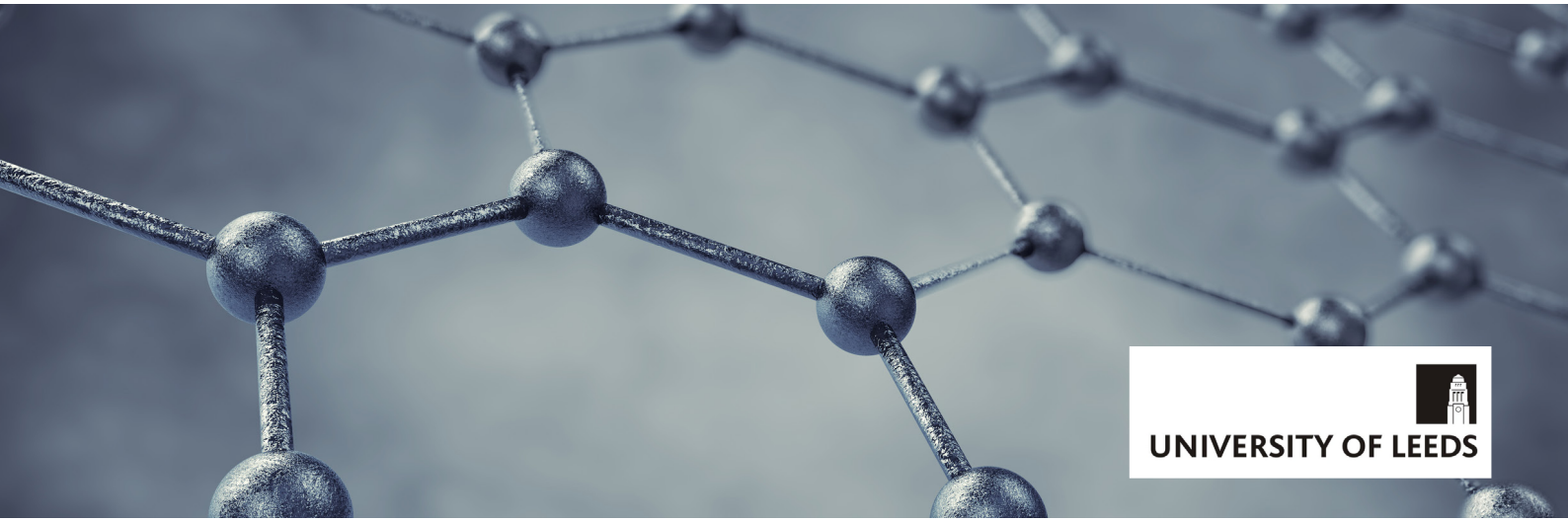
Accelerating the development of graphene

Hartree Centre
Science & Technology Facilities Council



The Institute for Materials Research at The University of Leeds has used the simulation capabilities of the STFC Hartree Centre to develop a better understanding of graphene for electronic applications.

Challenge

Flexible, strong and a good electrical conductor, graphene has vast potential as an interfacing material that could revolutionise the world of nanoelectronics. Current research is homing in on techniques to integrate graphene with other two-dimensional materials for use in future nanoscale devices. A successful future for graphene-based devices requires an understanding of its quantum mechanical behaviour – which means interpreting physical interactions at the atomic level. Aberration-corrected scanning transmission electron microscopy was used at SuperSTEM, STFC Daresbury Laboratory, to observe chemical bonding between metal contacts and graphene. The challenge was to provide a theoretical explanation of these observations.

Solution

In order to capture the subtle physical mechanisms taking place at the interface, the Hartree Centre provided the group from the University of Leeds with the intensive computational capability required to create accurate simulations. The simulated phenomena gave the scientists increased physical insight, predicting that metal dopants on graphene quickly migrate across the clean regions of the lattice and bond preferentially to edge sites and defects. This confirmed what they had observed using SuperSTEM, and allowed them to understand why it was happening at the atomic level. The results showed that graphene is chemically inert on its pristine regions, but highly reactive on edge sites and defects.

Benefits

A greater understanding of graphene will promote its potential future implementation into nanoelectronic circuits. This project allowed researchers to investigate how metal atoms bind or react with graphene, acquiring knowledge which will help to determine how graphene could work with metal contacts in electronic devices. Industrial applications include the potential for increasingly faster nanoelectronic technology in any device that uses a transistor, and improving the quality of solar cells. These applications could lead to cleaner, more efficient technology and boost UK competitiveness in electronics and associated high-tech fields.

"The Hartree Centre was vital to the success of our research. Without it, the project could not have been done – and not such a high standard. It is particularly useful to have access to both the HPC capabilities and expert support for the optimisation of code, enabling the machines to be used to maximum potential. It is also conveniently available a stone's throw from Manchester's new £61m National Graphene Institute."

– Andrew Scott, Institute for Materials Research, University of Leeds

Work with us

We collaborate with industrial clients and research partners on projects that create insights and value using high performance computing, big data analytics, simulation and modelling.

By combining our world-class facilities with access to our specialists and computational scientists, we can enable your organisation to produce better outcomes, products and services more quickly and cost-effectively than through conventional R&D workflows.

With our partners we are developing the next generation of supercomputing architectures and software, combining existing best practice with innovation to deliver faster, cooler and more sustainable solutions capable of meeting the challenges of data intensive computing.

For more information:

+44 (0)1925 603708
hartreecomms@stfc.ac.uk
@hartreecentre
/company/stfc-hartree-centre

VSN2