Thomas Mellan

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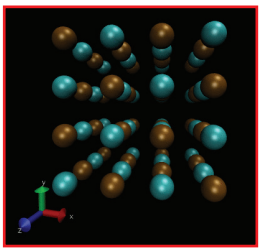
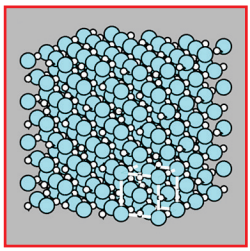
Thomas Mellan is a Post-Doctoral Research Associate in the Theory and Simulation of Materials at Imperial College London. He will use his prize to give an invited talk on his work on anharmonic vibrations in the USA, and intends to meet face-to-face with his collaborator at Argonne National Laboratory, with whom he has only corresponded by email. He will attend the 2018 American Physical Society March Meeting in Los Angeles, to present, and to meet US experts on ultra-high temperatures and anharmonicity.





As humans, we have an acute inbuilt sense of temperature. We instinctively know that below 0°C feels cold, and around 100°C is painfully the opposite.

Scientists and engineers, however, must consider temperature values far in excess of those we experience on a daily basis. In our research group, we compute the interactions between electrons and atoms. We use this data to model the properties of materials from 0 Kelvin all the way to thousands of degrees.

Our predictions are theoretical, but inform the material world. We attempt to answer difficult questions that have important consequences for our society, such as:

- How will the ceramic in the walls of a nuclear reactor behave in a melt-down event?
- Will the nose-cone material on a rocket crack or melt on re-entry?

Nuclear energy is a significant part of the UK's energy policy. It is critical that these plants are operated safely. Engineers therefore need to understand how the reactor will behave under different conditions. For example, they need to know how the cladding material will react to extremes of temperature - which cannot be measured using probes. We have been able to use our method to predict properties, such as thermal expansion and conductivity, of the cladding material.

Knowing this helps improve the safety and effectiveness of the plant.

ARCHER has enabled our calculations to predict the thermal properties of materials at temperatures up to 3800K. This has directly produced first-of-kind research on the vibrational properties of materials. We could not have done this using standard techniques.

Our group is part of a world-leading effort in understanding 'anharmonic' lattice vibrations. Using ARCHER allows us to match the standards of the best research groups in Germany and the US. Collaborating with these groups is very important for us and for the reputation of UK science worldwide.