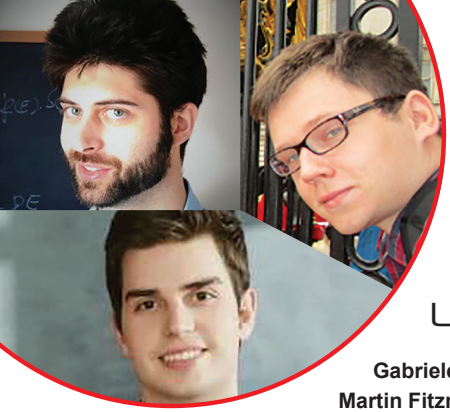
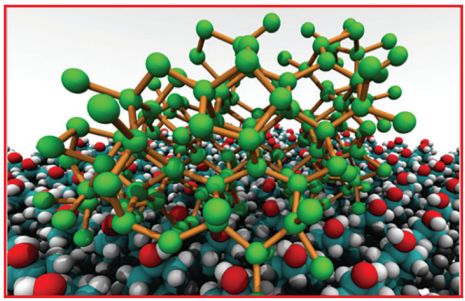


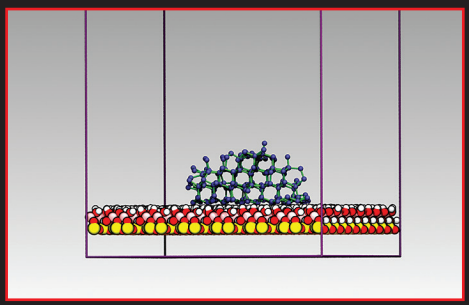
Gabriele Sosso, Martin Fitzner & Philipp Pedevilla

University College London

Gabriele Sosso is a postdoctoral research associate, and both Martin Fitzner and Phillipp Pedevilla are PhD students. They work in the Department of Physics and Astronomy at University College London, and are members of ARCHER's Materials Chemistry Consortium. With their prize, they plan to strengthen their existing collaboration with Shawn Kathmann at the Pacific Northwest National Laboratory Washington.



We use ARCHER to unravel the microscopic details of ice nucleation.



The formation of ice affects us every day - whether we are preserving food, curing disease, or understanding our weather. Understanding nucleation and growth, the processes which freeze water into ice, is critical. However, experiments looking at the formation of ice are incredibly challenging. This is due to the scales involved - on the order of nanometres and nanoseconds.

The simulations we have run on ARCHER give an unprecedented insight into the formation of ice on a molecular level. This knowledge can benefit both the academic community but also many aspects of industry.

In particular:

- Atmospheric scientists can take advantage of insights into ice formation. This will allow them to improve climate models, with important consequences for the fight against climate change.
- Cryobiologists in the Pharma, Biotech & Healthcare industries can use our research for a variety of purposes. This could be used to tailor and improve existing cryopreservation and cryotherapy techniques. This is due to the microscopic information we will provide about the effects of ice formation on biological matter.

Simulating ice is notoriously challenging, as it is very difficult to convince computer models of water to freeze. We have implemented enhanced sampling techniques to allow us to simulate ice formation. However, simulations of ice nucleation are still incredibly computationally expensive. This makes a facility like ARCHER invaluable. Using ARCHER allowed us to take advantage of massive parallelization. These kind of simulations cannot be done anywhere else within the UK, so ARCHER is just the right tool for the job.