Chiara Gattinoni

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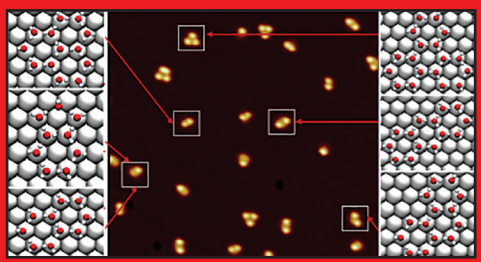
Chiara Gattinoni is a visiting researcher in the Tribology group at Imperial College London, and a post-doctoral researcher in the Department of Materials at ETH Zurich. With her prize, Chiara intends to visit the laboratory of Professor Charles Sykes at Tufts University in Massachusetts, and set up a joint collaboration between herself, Professor Sykes' group, and Dr David Prendergast of Lawrence Berkeley National Laboratory, to continue her previous work.

Water is everywhere: it covers 70% of the Earth's surface, it is present in air,and our bodies are about 65% made of it. At the microscopic scale, everything is covered in a thin layer of water. Understanding how water interacts with surfaces is very important to understanding the world around us. Interactions with water needs to be taken into account when building devices which might corrode. We can also exploit the interaction of water with surfaces for industrial purposes, such as renewable energy.



It is therefore very important that we understand how water behaves at interfaces. Despite great efforts by the scientific community, there is still a lot we don't know in this field.

In my work, I studied how water interacts with copper. I found new structures that water forms when it is in contact with a copper surface. ARCHER was used to compare simulations of water-copper systems with scanning tunnelling microscopy images.

In particular, we found that when a small number of water molecules are deposited on a copper surface, they form clusters. The clusters are generally composed of pentagons or hexagons, and the individual water molecules sit at different heights from the surface. The difference in height is clearly identifiable in the microscopy images as bright spots.

This discovery is a further step in the quest to understand the behaviour of water at the individual molecular level. More generally, this is the first step towards understanding corrosion, water splitting, and other industrially-relevant processes.

The use of ARCHER as a computational facility has been pivotal in the success of this project. The high-performance Cray nodes and high-speed interconnects enabled us to perform quantum mechanics calculations on large systems. We could not have simulated the water clusters without this capability.