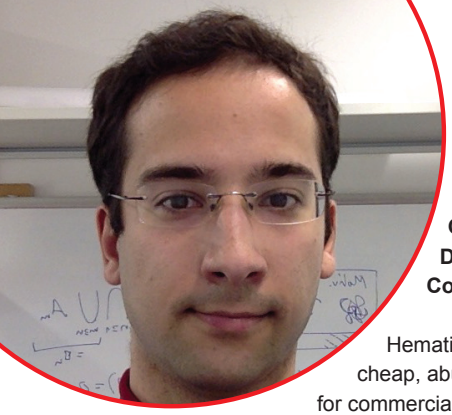
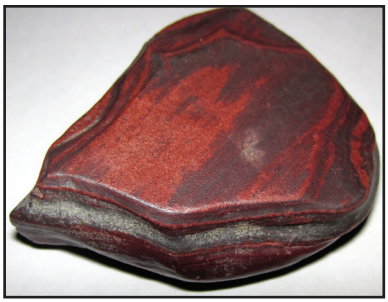


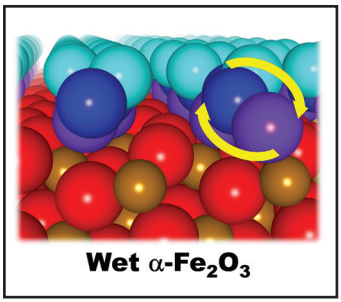
# Guido von Rudorff

## University College London

**Guido von Rudorff is a final-year PhD student in the Department of Physics and Astronomy at University College London.**

Hematite is one of the most common forms of iron ore. It is cheap, abundant, and non-toxic, which makes it a perfect material for commercialisation. Our work focuses on simulating the interface of hematite and liquid water, which is of interest in a wide range of fields. This interface is of particular interest in energy harvesting and storage.





**Wet $\alpha$-$Fe_2O_3$**

We already have a good understanding of both hematite in vacuum and solvent. However, to understand the full range of possible applications of hematite, we need to understand the interface of these two.

With the help of the Materials Chemistry Consortium and an ARCHER Leadership project, we assessed the interface using high-quality electronic structure calculations. This had not been done before and would not have been possible without ARCHER.

We simulated the hematite/water interface and measured the structural properties. At the same time, our collaborators' group in the USA measured the same properties experimentally. This way, we could compensate for the limitations of both approaches. The results of our research will enable better carbon-neutral energy harvesting. Moreover, our method is useful for a broad range of scientists. Many researchers in the computational chemistry and physics communities could benefit from our approach.

Our work is innovative, because we employ modern data analytics techniques to speed-up our research process. This is due to three grants by the cloud computing providers Microsoft Azure and Amazon AWS, as well as by the analytics company Tableau.

Our work demonstrates the capabilities of ARCHER to handle calculations of this size and computational load. Over 150,000 kAU were provided by an ARCHER Leadership project. We have shown that this UK resource enables significant scientific contributions of international interest.

As a result of this work, we have published four high-profile publications over the past three years. These have been well-received in the scientific community in the UK and overseas (including the USA). The methods we developed are implemented in our version of CP2K, the fourth most-used code on ARCHER.