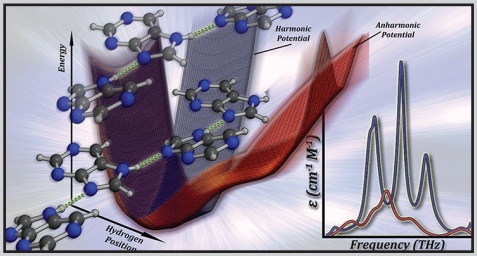
Michael Ruggiero

University of Cambridge

Michael Ruggiero is a postdoctoral research associate in the Department of Chemical Engineering and Biotechnology at the University of Cambridge. He plans to use his award to support his efforts to deliver his research to end users in the pharmaceutical community. He will present his research to the annual meeting of the American Association of Pharmaceutical Sciences, and visit collaborators in Pharmacy and Chemistry at the University of Minnesota.

Thanks to huge leaps in computational power over the past decade, our understanding of the quantum-mechanical properties of materials has been greatly enhanced. My research focuses on discovering the characteristics of solids using first-principles simulations. I use both experimental methods and simulations to predict and describe how solids behave in various conditions. My recent work has direct applications in the pharmaceutical, energy, and semiconductor industries.



A significant part of my research is investigating how temperature affects the properties of solids. I have used the CRYSTAL and CP2K codes to understand the very weak interactions in molecular crystals. These interactions are responsible for many observable phenomena.

Recently, I have been part of a study on disordered pharmaceutical solids. This has led to a significant advancement in the understanding of these materials' stability. This is a key factor in formulating new products that are safer and more cost-effective.

Without the ARCHER HPC facility, none of the work that I have done over the past year would have been possible. Accurately simulating disordered solids requires the modelling of a very large number of molecules. Traditional methods of simulating such large systems use classical molecular dynamics (MD) simulations. However, this method is unable to represent the complex interactions within the solid. Because of this, ab initio molecular dynamics (AIMD) has not been used to simulate large systems until very recently.

I have pioneered the use of AIMD to investigate the properties of solids. This has been used for both the crystalline and fully disordered states. Using CP2K, we have shown that AIMD simulations give the same results as experiments on crystalline solids. We have also found that these simulations can also be used for amorphous solids, with a high degree of accuracy. These results show that this technique can answer long-standing questions about amorphous solids. This includes questions such as the glass-transition problem, which has stumped physicists for over 60 years. This would not have been possible without the ARCHER facility, and the strong computational scaling of the CP2K code.