Alex Ganose

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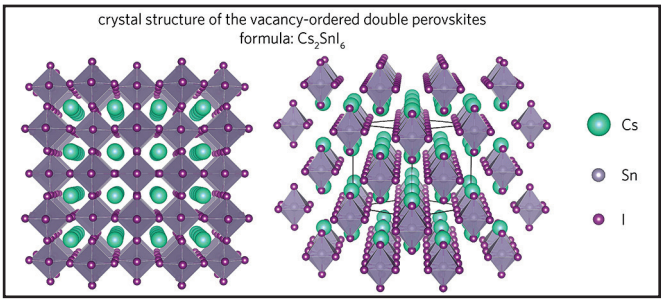
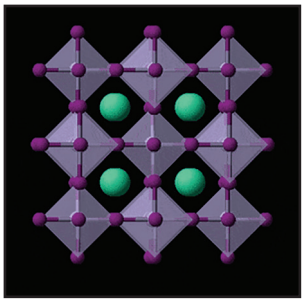
Alex Ganose is a 2nd year PhD student enrolled on the Molecular Modelling and Materials Science CDT program in the Department of Chemistry at University College London. He is a member of the ARCHER Materials Chemistry Consortium. With his prize, Alex plans to attend the 2018 spring meeting of the Materials Research Society in Phoenix, Arizona, and visit collaborators at Colorado State University.





Worldwide demand for energy is increasing all the time. Classic fuel sources, such as oil and gas, cannot keep up with this demand, and are harmful for the planet. Safe, renewable, economically viable energy sources are thus needed to fill the energy gap. The search for viable alternative fuels is the most pressing socio-economic concern faced by society today.

My work focuses on the search for new materials which can absorb energy form the sun. These can be used in 'photovoltaics' like solar panels. Solar energy is one of the most promising renewable energy sources as it is more-or-less unlimited, but the technology is far from perfect. New solar absorbing materials would improve the efficiency of solar cells. Using the latest computational chemistry modelling techniques, we can predict how a material will perform in a solar cell.

I have particularly been investigating one class of materials, the vacancy-ordered double perovskites. This class includes several promising candidates for new solar absorbers.

As part of this project, I have performed calculations on two members of the class, Cs_2SnI_6 and Cs_2TeI_6. Despite these two seeming very similar, they exhibit very different electrical conductivity. My calculations revealed that this is due to the behaviour of defects in the system. Based on this work, we have established the ideal conditions for optimising the electronic properties of Cs_2SnI_6. This will allow us to design new materials that do not have the same limitations.

This work was particularly challenging because of the complexity of these systems. Standard computational techniques are insufficient to accurately model the properties of these materials. Additionally, due to the size of the system, a large number of CPU cores is needed to complete the calculations in a reasonable time. For the most challenging properties, over 3,072 CPU cores were used for a single calculation. The scalability of compute resources, and the highly optimised computational chemistry packages available on ARCHER were instrumental in obtaining these results.