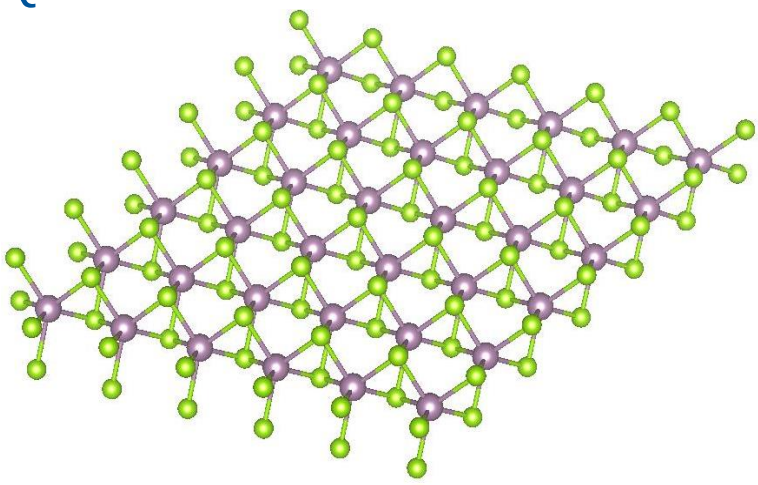
Case Study: N8 HPC and Lancaster University

Quantum Monte Carlo



Testimonial

"Quantum Monte Carlo (QMC) methods are known for their titanic computational requirements. These requirements necessitate access to large, reliable, and fast computer clusters capable of running parallel implementations of QMC methods. I have personally found the N8 HPC to be large enough for typical calculations to run acceptably, reliable enough to be able to "count on" jobs running and being completed before I desperately need their results, and fast. On a practical note, I have yet to experience a problem with: any of the pre-built modules, compiling applications, running jobs / using the queue system, and with accessing and using the file storage facilities. As far as clusters go, the N8 HPC is a pleasure to use."

Ryan Hunt - Department of Physics, Lancaster University

Project

Transition-metal dichalcogenides are atomically thin "two-dimensional" semiconductors closely related to graphene. These materials are currently being researched intensively by scientists around the world due to their fascinating optoelectronic properties and their potential for applications including photodetectors and high-speed field-effect transistors. Dr Neil Drummond's group at Lancaster University are using computer modelling to investigate these intriguing materials and providing the data needed to guide and explain current experimental work. To model these materials, quantum Monte Carlo techniques as implemented in the CASINO code (https://vallico.net/casinoqmc/) are being run on N8 HPC. Quantum Monte Carlo techniques use random sampling to find approximate solutions to the many-electron Schrödinger equation, which is the fundamental equation that governs the behaviour of the electrons in atoms, molecules and solids. Neil Drummond is one of the main developers of the CASINO code. A simpler approach for approximately solving the many-electron Schrödinger equation, called density functional theory, is also being used in some of the work.

Partners

Dr Neil Drummond – Department of Physics, Lancaster University
Dr Elaheh Mostaani - Department of Physics, Lancaster University
Dr Marcin Szyniszewski - Department of Physics, Lancaster University
Ryan Hunt - Department of Physics, Lancaster University

Success

Quantum Monte Carlo calculations are particularly well suited to massively parallel architectures such as N8 HPC, and the CASINO code has been shown to scale to tens of thousands of processor cores. The CASTEP code is being used for the density functional theory calculations. Both CASINO and CASTEP were straightforward to install and use on N8 HPC, with all required compilers and libraries being readily available. N8 HPC provides a stable platform for performing large numbers of quantum Monte Carlo calculations on up to 512 cores per job with good job-turnaround time. Without N8 HPC, the calculations would either have been done with substantially lower precision or with a critical delay of two or three months in the race to publish the findings in the globally competitive research field of two-dimensional materials.

Impact

There has been a great deal of controversy over the physical origin of peaks observed in the photoluminescence spectra of transition metal dichalcogenides, with apparently irreconcilable differences between experiment and theory. The quantum Monte Carlo calculations performed on N8 HPC have shown that these previously inexplicable peaks are due to complexes of five charges (e.g., two electrons and two holes bound to a charged defect). Such large charge-carrier complexes have not been considered or investigated in previous work. Armed with a more secure understanding of the physics underpinning the interaction of light with transition-metal dichalcogenides, experimentalists and theorists are now able to investigate more complicated devices and heterostructures of two-dimensional semiconductors.

N8 HIGH PERFORMANCE COMPUTING