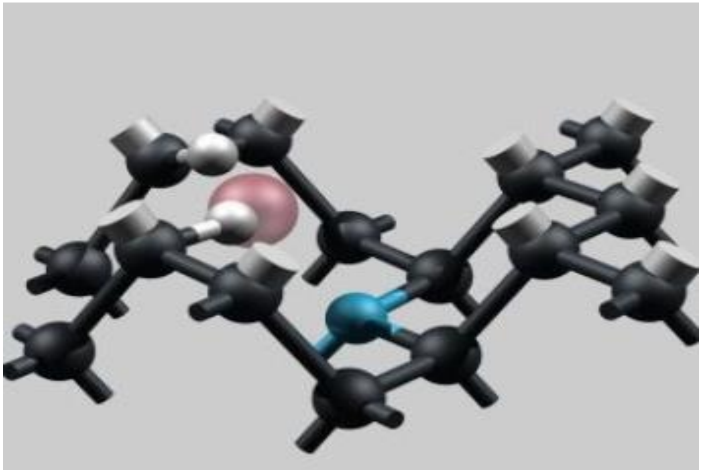
Case Study: Newcastle University and De Beers

Composition and Formation of Diamonds



Testimonial

"The very large number of simulations required to resolve these problems mean the progress could not have been made without the use of N8 HPC facility. All of the calculations were performed using our owns AIMPRO modelling code, which runs with a very efficient parallel scaling and can routinely simulate systems comprised of approximately 1000 atoms However, the use of a massively parallel computer system, such as Polaris, an N8 HPC machine, was critical to enable the use of quantum chemical codes such as AIMPRO."

- Professor Patrick Biddon, Newcastle University

Project

Polaris, the N8 High Performance computer, is being used to shed light on the composition and formation of diamonds.

First principle modelling calculations involving surfaces of crystals are particularly challenging as the processes are complex and require accurate, quantum-chemical simulations techniques. Since an accurate model of a surface must have sufficient surface area and depth to realistically represent a real diamond surface, the number of atoms required for even the simplest model make these calculations very demanding.

Partners

Professor Patrick Biddon – School of Electrical and Electronic Engineering, Newcastle University

Dr Jon Goss – School of Electrical and Electronic Engineering, Newcastle University

Dr Phillip Martineau – De Beers

De Beers

N8 HIGH PERFORMANCE COMPUTING

Impact

A better understanding and optimisation of the composition and formation of diamonds is key to more effective identification of the origins of diamonds, and differentiation between natural (geologically formed) and synthetic (man-made) diamonds.

It is also important for gaining a better understanding of advanced materials science which could be used in the development of low cost, high quality synthetic materials and technologies that could be used for novel applications in the fields of electronics, computing and advanced materials science.

Success

One of the defects the N8 HPC helped the team gain a better understanding of was the 'infrared' centre – which has defied identification for decades.

The formation process of this infrared centre in both geological and laboratory conditions points clearly to the key chemical reactions involved in the rearrangement of nitrogen in diamonds. The identification of the structure and composition of this is of great importance for connections between the gemmological use of diamonds, earth sciences and materials science, and a recently appointed PhD student, sponsored by De Beers, will be building further on this work to address a wide range of defect-related problems.