

We all experience pressure uniquely, and atoms are no exception! They aren't simple spheres as commonly thought. Using X-rays, we can reveal their intricate shapes and where their electrons are likely to be. This is achieved by analyzing a function known as electron density.

Through several calculus operations on electron density, we can pinpoint the boundaries of atoms, revealing their shape, size, and even their charge for ions. We aim to delve deeper into understanding atomic behaviour, particularly under extreme pressure conditions. This pursuit lies at the heart of this proposal.

Our objective is to apply immense pressure to minerals found in the Earth's interior, investigating how atoms morph and exchange charges under such conditions. To achieve this, we employ diamond anvil cells capable of generating pressures reaching hundreds of thousands of atmospheres on a single crystal of a mineral.

One intriguing finding we've encountered is that certain atoms seem to expand when subjected to pressure. This unexpected phenomenon arises from the flow of electron charge between atoms. We observed this effect in carbon atoms within calcite, a mineral commonly found in limestone formations (CaCO_3). Our next step is to expand our research to include a broader range of mineral groups, such as olivine, perovskite and apatite, to gain a comprehensive understanding of this intriguing phenomenon.

Perovskite, CaTiO_3 is a mineral with a fascinating crystal structure that holds great potential in modern technology. Its synthetic compositionally modified versions are being studied for use in renewable energy, particularly in the production of efficient and cost-effective solar cells. Due to its unique optical and electrical properties, perovskites could revolutionize the way we harness solar energy.

Apatite is a group of phosphate minerals that are incredibly important for life on Earth. It is the main component of the bones and teeth of all vertebrates. Its chemical formula is $\text{Ca}_5(\text{PO}_4)_3(\text{F}, \text{Cl}, \text{OH})$.

Olivine is a green mineral found in Earth's mantle and in meteorites ($(\text{Mg}, \text{Fe})_2\text{SiO}_4$). It's also used as a gemstone known as peridot. Our research will also focus on minerals that already have been transformed as a result of shock pressure, such as ringwoodite in meteorites, associated with impacts. Ringwoodite is a high-pressure polymorph of olivine, a common mineral in Earth's mantle. It forms under extreme pressure and temperature conditions typically found deep within the Earth.

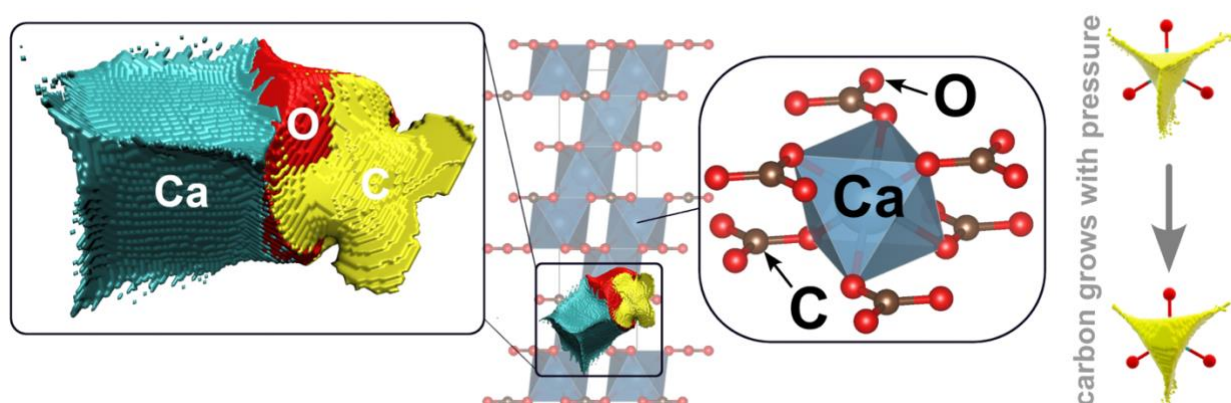


Figure 1. Fragment of the crystal lattice of calcite showing two representations of atoms. the view of atoms morphology (left). The classical polyhedral representation of atoms represented by spheres (middle). Example of carbon growth with increasing pressure from 8.5 to 11.3 kbar (right).