The ongoing developments of technology and improvements in facilities mean that using X-rays to explore the fine details of matter at the atomic level is growing in popularity. But as experiments become more sophisticated, so do results. Professor Oliver Kühn from the University of Rostock is working with fellow colleague Dr Sergey Bokarev to develop computational methods that will help researchers at the forefront of X-ray spectroscopy, analyse their results.

Deciphering the fingerprints of chemical bonds using X-ray spectroscopy

Whether you have broken an arm or suffered from a toothache, the likelihood is you have probably been X-rayed at some point in your life. As powerful beams of light capable of going through many substances, X-rays are not just useful for looking inside humans; they can be used to study the properties and structure of the molecular world, like the way atoms and molecules change during certain processes such as when a catalyst is used to increase the rate of a reaction.

X-ray science is becoming increasingly important because it is undergoing considerable change.

There are various ways matter can interact with X-rays, and as a result, various ways we can use X-rays. Molecules can diffract X-rays as they pass through, creating patterns typical for their structure. A famous example was the discovery of the DNA structure being a double helix by Watson and Crick. However, molecules can also absorb X-ray photons, promoting electrons to higher energy levels. Since X-ray photons have much shorter wavelengths than visible light, shining X-rays on molecules can be used to excite electrons that are bound close to the nucleus. As this is an unstable situation, the electron will fall back down, possibly emitting a photon at a different wavelength, which gives information complementary to absorption. Each atom has its own specific ‘X-ray fingerprint’, this means that X-rays can allow researchers to study materials and know exactly which elements they are looking at. This is a vital aspect as the function of enzymes and catalysts, for instance, is associated with changes in the electronic structure of specific atoms. In these examples, the relevant atoms are often metals containing many electrons interacting via Coulombic forces. Therefore, their motion is highly correlated, making the interpretation of X-ray spectra a complicated task.

For years, scientists have used synchrotrons to create high-energy X-ray photons. In recent years, however, there has been a shift towards using Free Electron Lasers (FELs) as a source of intense coherent X-ray light. A prominent example being the XFEL in Hamburg (Germany), which has now been officially opened.

These light sources provide insight into the structure of matter at an unprecedented level of detail. Therefore, the results of X-ray absorption and emission experiments can be rather complex to decipher and require a parallel development of novel computational models. Being part of a worldwide activity of theoretical physicists
What are X-rays biggest ‘rivals’ when it comes to studying the electronic structures of matter?

Traditional spectroscopy in the visible or ultraviolet regime has been developed to a high sophistication. Its focus is on valence electrons, whose density is usually smeared out over the whole molecule. In contrast, X-rays are unique for probing local changes in electron delocalisation e.g. during a chemical reaction. In terms of the X-ray sources, large-scale facilities like XFELs are competing with tabletop so-called ‘high-harmonic generation’ setups in the soft X-ray regime.

What is it important to know how electrons behave in atoms and compounds?

Electrons are the glue that holds molecules together. Hence analysing the electron density distribution is key to understanding chemical bonding as well as bond breaking and formation during chemical reactions. On the other hand, the transfer of electrons between molecules is at the heart of many processes, ranging from corrosion and catalysis to photosynthesis.

Why are you personally interested in the subject?

Clearly, X-ray spectroscopy provides extremely detailed insight into fundamental processes across the disciplines of natural sciences. The combination with high time resolution is likely to reshape our way of thinking about these processes and the underlying concepts in the near future. From the theory side, studying the intricate many-body dynamics of electrons and nuclei is simply just a fascinating endeavour.

Do you think synchrotrons or free electron lasers will be the future of X-ray spectroscopy?

Synchrotron sources are well-established and have a prominent place in scientific investigations. Free electron lasers open up a new direction, with a strong focus on time-resolution. In a way, these are complementary experiments, which will coexist for a mutual benefit.

What are the big questions you’re hoping to answer through your research in the next couple of years?

The interaction of matter with X-rays also leads to the ejection of electrons leaving the molecules ionised. The characteristics of these electrons yield information which is complementary to photon emission. The power of simultaneous analysis of these emission events has yet to be explored. Furthermore, understanding the interplay between different electron-out channels is one of the key challenges that will be tackled by our group.

The future of X-ray science is in time-resolution using extremely short flashes of X-rays, this process can be controlled despite overwhelming decay channels, and the flipping time substantially reduced.

This research is opening new doors when it comes to X-ray science, allowing researchers across the world to probe increasingly complex processes. As the technology to produce X-rays continues to improve, the methods developed by Prof Kühn and his team will enable researchers across different disciplines, to further our understanding of how functional materials work on the atomic scale. Progress on the simulation side is expected to come with the emerging quantum computers, which will further push the limits to an extent not foreseen by the founding fathers of quantum mechanics.