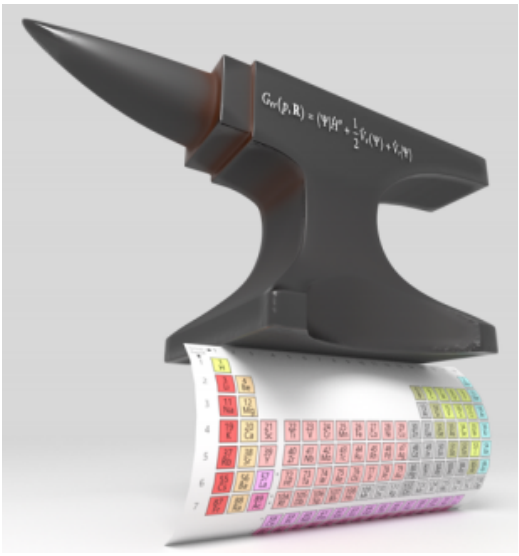
Squeeze your Chemical Imagination: Bonding in Extreme Conditions



Chemistry is dramatically different under conditions of high pressure. The structure of the periodic table itself changes. Properties of atoms, as size, electronegativity, and electron configuration [1] are drastically reordered. The application of pressure can be used to create entirely new chemical species and materials with odd properties. For example, noble gas elements can be made to react, core electrons can be made to partake in bonding, conductivity can be created in a host of materials and near-room temperature superconductivity has been achieved [2,3].

The necessary pressures are often millions of times higher than atmospheric, *i.e.* above 100 GPa, but can today routinely be created in laboratories. However, experimental techniques are costly and time consuming and have only scratched the surface of what might be discovered in the high-pressure regime. Predictions from quantum mechanical calculations are today essential for guiding experimental efforts, and that is the focus of this project. One important question is whether we can learn to tune bonding in molecules and materials by compression, so to reach electronic states and properties that one cannot envision at ambient conditions.

Project description

You will learn to study and predict molecular properties under extreme conditions of pressure using quantum chemistry calculations. The general aim of the research is to explore the potential for new chemistry. There exist several possible research directions, for example:

- Systematically study the effect of pressure on molecules using a novel computational method
- Apply and evaluate a new method that computes electronegativity of atoms inside materials
- Explore the role of pressure on chemical reactivity

Learning outcomes

By working on this project, side by side with Chemistry researchers, you will learn how to:

- Use state-of-the-art quantum chemistry codes
- Work with high performance computing environments.
- Understand and resolve chemical problems in non-conventional conditions.
- Develop critical thinking, and learn to present scientific results both written and oral form.

About the group

You will be involved in a multidisciplinary group with physicists, chemists, and engineers in an international environment (www.rahmlab.com). Our scientific interests include astrochemistry, chemical bonding, high pressure, and quantum computation. You will join weekly meetings where we share and discuss our take on problems at hand and recent scientific trends.

Literature tips and References

[1] “Squeezing All Elements in the Periodic Table: Electron Configuration and Electronegativity of the Atoms under Compression.” https://doi.org/10.1021/jacs.9b02634
[2] “The Chemical Imagination at Work in Very Tight Places.” https://doi.org/10.1002/anie.200602485
[3] “Chemistry under high pressure.” https://doi.org/10.1038/s41570-020-0213-0

Contact details

Martin Rahm (room 5019, Chemistry building 1): martin.rahm@chalmers.se