

The Research Group
General Chemistry

has the honor to invite you to the public defence of the PhD thesis of

Jochen Eeckhoudt

to obtain the degree of Doctor of Sciences

Title of the PhD thesis:

**Electronic Structure and Reactivity at High Pressure
using Hydrostatic Pressure Models**

Supervisors:

Prof. dr. Frank De Proft (VUB)

Prof. dr. Mercedes Alonso Giner (VUB)

The defence will take place on

Thursday, December 11, 2025 at 4:30 p.m.

VUB Etterbeek campus, Pleinlaan 2, Elsene,
auditorium I.O.03

The defence can be followed through a live
stream: [Click Here](#)

Members of the jury

Prof. dr. Ulrich Hennecke (VUB, chair)

Prof. dr. Charlotte Martin (VUB)

Prof. dr. ir. Freija De Vleeschouwer (VUB)

Prof. dr. Wim Vranken (VUB)

Prof. dr. Eduard Matito (DIPC/Ikerbasque Foundation for
Science, ES)

Prof. dr. Tim Neudecker (University of Bremen, DE)

Prof. dr. Martin Rahm (Chalmers University of
Technology, SE)

Curriculum vitae

Jochen obtained his Ba in chemistry at the VUB in 2019 and his Ma in 2021. Next, he pursued a doctorate by continuing his research into high pressure chemistry and was supported by an FWO fundamental research fellowship. During his Ph.D. he published two first author publications and is in the process of publishing four additional papers. He attended 8 international conferences and presented his work in both poster sessions and an oral communication at the Young Research Symposium of CBOND2024. Besides his research, Jochen supervised 5 student theses and taught numerous exercise and lab sessions. Finally, he represented the OAP staff of his faculty in various university committees.

Abstract of the PhD research

High pressure chemistry is an interdisciplinary subfield of chemistry and physics with a long and rich history spanning over a century. It has provided numerous advancements in the fields of chemical synthesis, superconductivity, superhard materials and other exotic chemical compounds. Modelling reactions and materials at the pressures that are encountered at the bottom of oceans and cores of planets has played an important role in many of these discoveries. In recent years, new models that allow for a quantum mechanical description of molecules under pressure have been developed and these models are used in this work to study several aspects of high pressure chemistry. First, the chemical concepts such as electronegativity and chemical hardness are studied at high pressure by extending the conceptual density functional framework. These are shown to already explain several observations encountered in the high pressure world. Next, several models to impose pressure on molecules are meticulously compared against each other for the first time. The results stress the importance of a proper description of the boundary between the molecule and the pressurizing medium. A more theoretical section then attempts to derive an equation for and subsequently compute the change of the dipole moment of molecules when the pressure increases. As a step towards larger molecules, the aromaticity concept is investigated under pressure for benzene, leading to several recommendations to the community. Finally, the ring opening reaction of Dewar benzene is studied and it is shown that reaction properties accessible through high pressure experiments can be matched to theory in order to better understand the underlying mechanism. As an epilogue, cation- π interactions between the side chains of amino acids in proteins are studied using a combined statistical and theoretical approach. This revealed that the perceived prevalence and importance of these interactions might be overstated.