SCIENCES &
BIOENGINEERING SCIENCES

The Research Group
General Chemistry
has the honor to invite you to the public defence of the PhD thesis of

Charlotte Titeca

to obtain the degree of Doctor of Sciences

Joint PhD with KU Leuven

Title of the PhD thesis:

Computational and Conceptual Density Functional Theory for Electronic Resonances

Supervisors:

Prof. dr. Thomas-C. Jagau (KU Leuven)
Prof. dr. Frank De Proft (VUB)

The defence will take place on

Tuesday, October 14, 2025 at 5 p.m.
in Justus Lipsiuszaal, Erasmushuis,
Blijde-Inkomststraat 21, 3000 Leuven.

Registration and livestream:
https://forms.office.com/e/88bpu3QV4L

Members of the jury

Prof. dr. Alessandro Ianiro (KU Leuven, chair)
Prof. dr. Mercedes Alonso Giner (VUB)
Prof. dr. Daniel Escudero (KU Leuven)
Prof. dr. Luc Van Meervelt (KU Leuven)
Prof. dr. Nigel Mason (University of Kent, UK)

Curriculum vitae

Charlotte Titeca obtained a Master degree in Chemistry in 2021 from KU Leuven, during which she had already been active at VUB as internship student in the research group of General Chemistry. After her master thesis about the solvation of anions, for which she received the Chemici Leuven Prijs, she started a joint PhD at KU Leuven and VUB as FWO fellow. Here, she combined the theoretical description of unbound electrons with conceptual density functional theory. Charlotte published two articles as first author and a third article as co-author. Moreover, she showcased her work by means of a poster or a presentation in eight international conferences and completed a research stay in California. Additionally, she guided exercise sessions for first-year students and made her research known to the wider public through an Eos blogpost.

Abstract of the PhD research

The research presented in this thesis is aimed at obtaining increased insight into molecular processes involving compounds containing unbound electrons, so-called electronic resonances. For this purpose, quantum chemical methods are employed, more specifically density functional theory. This is a versatile method allowing calculation of the energy and the properties of a wide range of systems at reasonable computational cost, as well as understanding the bonding patterns and reactivity of molecules. Particular attention is paid to dissociative electron attachment, taking place when electron attachment to a stable molecule results in formation of an electronic resonance undergoing bond breaking. This process is ubiquitous and occurs for instance in DNA after exposure to radiation, and is as such exploited for treating cancer using radiotherapy.

The presence of an unbound electron requires the use of adapted techniques. In the current work, two different approaches are applied: charge stabilization and addition of a complex absorbing potential. In the former method, the molecule is artificially modified such that the unbound electron becomes bound and can be treated using the conventional quantum chemical methods. We present an extension of the original charge stabilization method beyond the calculation of energies, reporting on its application for obtaining the electron localization function that shows were the unbound electron is localized. This allowed us to develop an approach for predicting whether dissociative electron attachment will occur and which bond(s) will be most affected.

Next, we directed our attention to molecules with a cage-like structure that are hypothesized to catch an electron inside the cage. The bound or unbound character of the excess electron depends on the specific method used for describing these molecules. We applied our extension to charge stabilization to investigate whether the electron is really located in the cage and how its description varies among different methods.

In the final project, the complex absorbing potential was considered. It acts like a wall preventing the unbound electron from leaving the system. Combinations of this approach with density-based methods are very scarce in scientific literature and software. We describe our implementation of complex absorbing potentials for density functional theory and report on the first results obtained using this promising method.