SCIENCES & BIOENGINEERING SCIENCES

The Research Group

General Chemistry

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

Tatiana Woller

to obtain the degree of Doctor of Sciences
Joint PhD with Sorbonne Université

Title of the PhD thesis:

Design of Molecular Switches Based on Expanded Porphyrins: Computational and Conceptual Aspects

Promotors:

Prof. dr. Frank De Proft
Prof. dr. Mercedes Alonso
Dr. Julia Contreras-García

The defense will take place on

Tuesday, August 31, 2021 at 16h00

and can be followed online through a live stream. Please contact Tatiana.Woller@vub.be for more information.

Members of the jury

Prof. dr. Ulrich Hennecke (VUB, chairman)
Prof. dr. ir. Freija De Vleeschouwer (VUB, secretary)
Prof. dr. ir. Vincent Ginis (VUB)
Dr. Vanessa Labet (Sorbonne Université, FR)
Prof. dr. Monica Calatayud (Sorbonne Université, FR)
Dr. Eduard Matito (Donostia Int. Physics Center, ES)
Prof. dr. Gabriel Merino (Centro de Investigación y de Estudios Avanzados, MX)

Curriculum vitae

Tatiana Woller obtained the degree of Master of Science in Chemistry at the VUB in 2015. Afterwards she started as a teaching assistant and PhD student in the Department of General Chemistry, VUB. A fruitful Erasmus exchange led to a joint PhD with Sorbonne Université.

During her PhD she studied the potential of expanded porphyrins as molecular switches. In the meantime, she published 11 articles in peer-reviewed international journals. Finally, the PhD involved teaching tasks encompassing the supervision of two bachelor and one master students.

Abstract of the PhD research

The design of molecular switches opens exciting paths towards practical applications, such as molecular sensors for monitoring heavy metal ions or as photocatalysts to functionalize aldehydes. Among molecular machines, molecular switches can adopt at least two states encoding for distinct properties in response to external *stimuli*.

With their versatile topology and properties, expanded porphyrins can act as a molecular switch. Nevertheless, those macrocycles are challenging to study due to their extensive size and their aromaticity. As it is associated to many properties, aromaticity holds a pivotal place in the chemistry of porphyrins. This PhD aims at designing molecular switches based on expanded porphyrins using a conceptual and a computational approach.

This PhD work is subdivided in a methodology and in an applied part. The methodology part concentrates on assessing which method is suitable to study the energetic aspects and electronic properties of such macrocycles. Given the complexity of expanded porphyrins, the assessment of the method to study the properties is a tedious task. In the second part, we explore the connection between the photophysical properties, the aromaticity and the topology of expanded porphyrins in various states (neutral, anionic, cationic and core-modified). In general, the aromaticity leaves its fingerprint on absorption spectra of expanded porphyrins but it is not the only factor determining the patterns of absorption spectra. By contrast, the magnitude of the nonlinear optical properties is connected to geometrical parameters. This work offers proof that expanded porphyrins can act as efficient molecular switches.