SCIENCES & BIOENGINEERING SCIENCES

The Research Group

General Chemistry (ALGC)

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

Thijs STUYVER

to obtain the degree of Doctor of Sciences

Title of the PhD thesis:

Qualitative Insights into the Transport Properties of Molecular Electronic Devices: A Quantum Chemical Approach

Promotors:
Prof. dr. em. Paul Geerlings
Prof. dr. Frank De Proft
Dr. Stijn Fias

The defence will take place on

Wednesday May 30 2018 at 17.00h

in Auditorium D.2.01 at the Campus Humanities, Sciences and Engineering of the Vrije Universiteit Brussel, Pleinlaan 2 - 1050 Elsene, and will be followed by a reception.

Members of the jury:

Prof. dr. Steven Ballet (chairman)
Prof. dr. Frederik Tielens (secretary)
Prof. dr. Dominique Maes
Prof. dr. Jan Danckaert
Prof. dr. Roald Hoffmann (Cornell University, USA)
Prof. dr. ir. Veronique van Speybroeck (Universiteit Gent)
Prof. dr. Benoît Champagne (Université de Namur)

Curriculum vitae

Thijs Stuyver (°1992) graduated as Master of Science in Chemistry at the VUB in 2014. Subsequently, he started his PhD on the topic of molecular electronics. His research was funded by the FWO through an aspirant fellowship. During his PhD, he stayed 3 months at Cornell University, USA (NY). His research has resulted in 12 publications in international peer-reviewed journals, of which 8 as first author. He supervised a bachelor thesis and presented his work at (inter)national conferences. Thijs was also involved in many of the governing bodies of the university as a representative.

Abstract of the PhD research

Single-molecule electronics, the study of the electrical transport through single molecules connected in a circuit, can be considered as the ultimate step in the down-sizing of electronic components and thus carries great technological potential. However, chemical understanding of the transport properties of molecules is still rather limited. This provides an impetus for theoretical and experimental chemists alike to investigate the phenomena associated with electric transport through molecules and the influence of the structure of these molecules on them.

Starting from the so-called Source-and-Sink Potential model at Hückel level of theory, an expression for the transmission probability of electrons through a molecule was obtained and cast in a graph-theoretical form. Clear structure-property relationships for the electric transport through molecules were obtained and connected to chemical concepts. With the help of the derived structure-property relationships, the occurrence of quantum interference – leading to an extremely low current when a small voltage is applied – could be predicted based on the structure of the molecule. Additionally, several guiding principles were formulated for tuning the conductivity of molecules, either through geometrical changes, through changes in the aromaticity patterns or through substitution.

With all of these tools at hand, a wide range of applications were considered throughout this thesis. We explored the switching properties of a number of light-, redox- and heat sensitive molecules, among which expanded porphyrins. Additionally, we investigated a wide range of molecular wires and all the different ways to make them more/less conducting. Furthermore, the paths the current takes through conjugated molecules has also been studied and a strategy was devised to "seal off" part of the molecule for this current. Finally, we contributed to the further development of the Source-and-Sink Potential formalism, by developing a computer code capable of visualizing the path the current takes through the molecule in real space at higher levels of theory (Hartree-Fock and Density Functional Theory).

Our results will hopefully guide experimentalists in their quest for the design of optimal functional electronic components at the single-molecule-level.