SCIENCES & BIOENGINEERING SCIENCES

The Research Group
ALGC/SUME

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

Lise Vermeersch

to obtain the degree of Doctor of Sciences

Title of the PhD thesis:
Breaking Down the Building Blocks: Computational Exploration of Sustainable Covalent Adaptable Networks Based on Diels-Alder Chemistry

Supervisor:
Prof. dr. ir. Freija De Vleeschouwer (VUB)
Co-supervisor:
Prof. dr. Niko Van den Brande (VUB)

The defence will take place on

29th of May, 2026 at 5 p.m.

VUB Etterbeek campus, Pleinlaan 2, Elsene, at the LIC, room LIC LT.

Members of the jury

Prof. dr. Frank De Proft (VUB, Chair)
Prof. dr. Mercedes Alonso (VUB)
Prof. dr. Cathy Macharis (VUB)
Prof. dr. ir. Guy Van Assche (VUB)
Prof. dr. Thijs Stuyver (PSL University in France)
Prof. dr. Jelle Vekeman (University of Antwerp)

Curriculum vitae

Lise Vermeersch obtained a Bachelor's degree in Architectural Engineering in 2018 and subsequently completed both a Bachelor's and Master's degree in Chemical Engineering at Vrije Universiteit Brussel. Since 2021, she has been pursuing a PhD in Quantum and Computational Chemistry, where her research focuses on the computational modelling of sustainable self-healing materials using approaches ranging from density functional theory to molecular dynamics simulations. Her doctoral research is supported by an FWO fellowship and has been complemented by an international research stay at Pennsylvania State University, alongside contributions to interdisciplinary sustainability research and academic mentoring.

Abstract of the PhD research

Many modern polymers are strong and lightweight but difficult to repair or recycle. A promising solution is the use of chemical reactions that can form and break bonds in a controlled way. The Diels–Alder reaction enables materials that can heal themselves, be reshaped, or be recycled. This thesis explores how these reactions can be better understood and optimized to design more sustainable materials. Using computer calculations, a wide range of Diels–Alder reactions were studied to identify trends in reaction speed and stability. The results were collected in a database, and machine learning was evaluated as a fast way to predict promising reactions without the need for extensive calculations. In addition, the work investigates how Diels–Alder reactions can be accelerated using catalysts, with a focus on weak, reversible interactions that enhance reaction rates without compromising the material's ability to heal and be recycled. Because large molecules are flexible and can exist in multiple shapes, this thesis introduces BoltCAR, a computational tool that accounts for all relevant molecular conformations and their contribution to overall reaction behavior. These molecular insights are then linked to larger-scale simulations of polymer formation and behavior, and validated through laboratory experiments. Finally, the thesis proposes a practical framework to assess whether new material concepts are not only scientifically sound but also environmentally and socially responsible before further development.