

Doctor of Engineering Physics (Ghent University, 2026)

MSc Engineering Physics (Ghent University, 2019)

Experienced researcher in computer-aided modelling of (nano)materials looking for challenges in R&D, modelling and optimisation in engineering fields. Punctual and detail-oriented setup and execution of both theoretical and applied research projects.

EXPERIENCE Researcher (Sep 2019 – Aug 2026) Center for Molecular Modeling

Dissertation: *Bridging the Gap between Computational and Experimental Nuclear Magnetic Resonance Spectroscopy in Nanostructured Materials* (2026).

Promoters: prof. dr. ir. Veronique Van Speybroeck (UGent) & dr. ir. Eric Breynaert (KU Leuven)

Combining physics, quantum chemistry and materials science to understand the atomic structure of crystalline materials relevant to the chemical industry through the use of nuclear magnetic resonance spectroscopy and molecular modelling.

Close collab with diverse partners (KU Leuven, UGent, UAntwerpen, Umicore).

Teaching Assistant (Oct 2021 – Aug 2026) Department of Applied Physics

Education of physics and mathematics in the Bachelor of Engineering (UGent).

EDUCATION Doctoral Study Programme (2019 – 2026) Doctoral Schools, UGent

Specific courses: *Education Programme for Assistants, Mind the GAP: Good Academic Practices, Materials Chemistry & Physics, Winter School for Theoretical Chemistry and Spectroscopy (exchange).*

MSc Engineering Physics (2017 – 2019), *cum laude* UGent

Civil Engineering programme: Engineering Physics. Focus on both theoretical and applied physics.

- ## SKILLS
- Analytical insight, translating research goals into results for materials science, bringing together multidisciplinary research results in scientific publications.
 - Theoretical design, application and optimisation of workflows and molecular models.
 - Coordinating with experimental partners and industry to translate industrial needs to research objectives.
 - Analysis of experimental and computational spectroscopic and crystallographic data.
 - Executing and supervising research projects including supervising two MSc thesis students, technical and general reporting to stakeholders (academic and industrial).
 - Presenting and public speaking: talks at conferences, plenary exercise class lectures, structured progress reports of projects.
 - Education of mathematics and physics courses, formulating exams and homework and correcting, individual and group feedback.
 - Languages: Dutch (mother tongue), English (full), French (working), German (basic).
 - Software/programming: Python, bash, git, Maple, Matlab, CP2K, QuantumEspresso, VASP, ORCA, Gaussian, Atomic Simulation Environment.

SELECTED
PUBLICATIONS,
CONFERENCES

- Article: *Computational Protocol for the Spectral Assignment of NMR Resonances in Covalent Organic Frameworks*
Vanlommel, S., Borgmans, S., Chandran, V. C., Radhakrishnan, S., Van Der Voort, P., Breynaert, E., Van Speybroeck, V.
Journal of Chemical Theory and Computation, **2024**, 20, 9, 3823–3838.
- Article: *How Water and Ion Mobility Affect the NMR Fingerprints of the Hydrated JBW Zeolite: A Combined Computational–Experimental Investigation*
Vanlommel, S., Hoffman, A.E.J., Smet, S., Radhakrishnan, S., Asselman, K., Chandran, V. C., Breynaert, E., Kirschhock, C.E.A., Martens, J., Van Speybroeck, V.
Chemistry – A European Journal, **2022**, 28, e202202621.
- Article: *Hindered Dynamic Diversity: NMR Investigation of Cation Species in Zeolite Growth Systems*
Vanlommel, S., Chandran, V. C., Temmerman, W., Vandenabeele, D., Kirschhock, C.E.A., Breynaert, E., Verstraelen, T., Van Speybroeck, V., Vekeman, J.
Under review.
- Article: *Deciphering Framework Aluminium in Zeolites via a Convergent Computational–ssNMR Strategy: The Case of Chabazite*
Vanlommel, S., Chandran, V. C., Smet, S., Vanbutsele, G., Hoffman, A.E.J., Martens, J., Radhakrishnan, S., Breynaert, E., Van Speybroeck, V.
Under review.
- Talk: *Challenges in simulating aluminosilicate zeolites and connecting NMR theory to experiment*
Smarter8, September 2024, Aveiro, Portugal.
- Talk: *Computational NMR as an asset to structural investigation of complex materials*
Smarter7, September 2023, Leuven, Belgium.
- Talk: *How water and ion mobility affect the NMR fingerprints of the hydrated JBW zeolite*
Winterschool for Theoretical Chemistry and Spectroscopy, November 2022, Han-sur-Lesse, Belgium.

Full list of publications and conference contributions:
molmod.ugent.be/members/siebe-vanlommel

AWARD Young Scientist Award – International Union of Crystallography (2024).