

**Modeling functional nanostructured materials for future technologies at the intersection of quantum mechanics, statistical physics and machine learning**

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Our society faces significant challenges, such as how to provide an affordable and clean energy system without endangering future generations, how to protect our limited natural resources, how to combat environmental pollution, how to mitigate climate change. Functional nanomaterials are crucial in developing future technological solutions to address these questions. Ideally nanomaterials can be designed with atomic scale precision to provide the desired macroscopic function. From a purely experimental basis, it is extremely difficult to establish a causal relation between nanometer scale structural modifications and the observed macroscopic function of the material. However, modeling functional nanomaterials in close synergy with experiments can provide this nanoscopic insight, provided it yields a realistic nanometer-scale representation of the functional material.

Such modelling of realistic functional nanomaterials poses significant challenges. First of all, nanostructured materials used in applications are far from perfect, they possess a broad range of heterogeneities in space and time extending over several orders of magnitude. Spatial heterogeneities from the subnanometer to the micrometer scale in crystal particles with a finite size and specific morphology, impact the material's dynamics. Furthermore, the material's functional behaviour is largely determined by the operating conditions. Currently, there exists a huge length-time scale gap between attainable theoretical length-time scales and experimentally relevant scales.

In this talk, I will demonstrate how modeling at the intersection of quantum mechanics, statistical physics, and machine learning, in synergy with experimental work, has advanced to the point where designing functional nanomaterials for critical technologies is now possible. The concepts will be made clear by timely applications in the fields of sustainable chemistry, clean energy and nanosensing. Applications encompass materials to convert non-fossil based feedstocks to platform chemicals, to capture CO<sub>2</sub>, to harvest water from the air in dry areas or to capture volatile organic compounds to provide clean air. Modeling of realistic nanomaterials requires a multidisciplinary vision between physics, chemistry, material science, engineering and machine learning.

Biosketch Prof. Veronique Van Speybroeck
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Veronique Van Speybroeck is full professor at the Ghent University and head of the Center for Molecular modeling (<http://molmod.ugent.be>), a multidisciplinary research center composed of about 40 researchers. She was trained as an engineer in Physics and obtained her PhD in 2001 from the Ghent University. She has a record of [significant contributions](#) in the field of modeling nanoporous materials for catalysis, adsorption; all applications are inspired and performed in close synergy with experimental groups. The research is driven by the ambition to model as close as possible realistic materials/processes and systematically pushed the limits of simulation methods. She developed methods to calculate chemical kinetics for reactions taking place in nanoporous materials and pioneered the simulation of complex catalytic cycles at operating conditions using enhanced sampling molecular dynamics methods. Currently, she is exploring methods to resolve complex catalytic cycles bridging length and time scales. She was recipient of two ERC grants, received numerous recognitions and prizes, such as the [Dr. Karl Wamsler innovation award in 2023](#) and the [Francqui prize in exact sciences](#) in 2024. She is also an elected member of the Royal (Flemish) Academy for Science and the Arts of Belgium (KVAB, [www.kvab.be](http://www.kvab.be)).

She lectures various Master and Bachelor courses within the Faculties of Engineering and Sciences in the field of *Atomic and Molecular Physics, Molecular Modeling of industrial processes, Chemistry of Industrial Processes, Advanced Quantum Mechanics*