Namur Institute of Structured Matter (NISM)

The **Namur Institute of Structured Matter** research interests cover various topics in the field of **organic and physical chemistry**, **materials chemistry, surface science, solid-state chemistry and physics** from both **a theoretical and experimental** point of view.

NISM enables the exchange of ideas and competences in the field of synthesis and functionalization of molecular systems and novel materials (0D, 1D, 2D and 3D), the rational design of solids with specific architecture and surface properties as well as the development of advanced techniques for the study of their physicochemical properties. An important role is played by the theoretical approaches, through numerical simulation and modelling, which contribute to the development of new materials (synthesis, structure, growth) as well as to the prediction of their properties.

The applications involve a broad range of research areas including photonics, nonlinear optics, (photo)catalysis, plasma physics and chemistry, inhibition of viral and/or bacterial pathogens…

1. Nonlinear Optics and Photonics

Research is carried out in nonlinear optics (NLO), quantum NLO, plasmonics, and photonics, applied to multiscale structured matter (i.e. molecules, surfaces, biomaterials, nanomaterials, metamaterials, and crystals). Optical responses and their coupling to vibrational and electronic excitations are predicted, from theoretical models using numerical simulations, and measured, using dedicated experimental setups, with the goal to better understand light-matter interactions in nature or in artificial systems, and to optimize their effects in view of technological applications.

2. High Performance Computing (HPC) Multiscale Modelling

The HPC pole aims at 1) sharing computational techniques, skills and tools in order to develop new materials and predict their final properties and 2) improving the modelling techniques and computer codes to account for most of the chemistry and physics of structured matter.

3. Functional Structured Materials

The core of our expertise is divided in two interconnected areas:

1) The development of 3D porous architectures including hierarchical organizations, MOF or MOF-like systems, biologic, organic/inorganic hybrids both using silica and carbon- based media, nanocomposites…
2) The functionalization of nanostructures such as carbon nanotubes, fullerenes (C_{60}), pillar-arenes, silsesquioxanes (POSS)...

The applications cover various hot topics including: Li-batteries, CO_2 conversion, biomass conversion, photosynthesis, (photo)catalysis, inhibition of viral and/or bacterial pathogens, biomaterials, sensors…

4. Surfaces, Interfaces and Carbon Nanostructures

Synthesis, characterization and modelling of novel materials, with particular attention to interfaces between two distinct phases and to low-dimensional structures including carbon nanostructures (graphene, nanotubes). A large choice of deposition and characterization methods is available within the **SIAM** technology platform. A strong theoretical support is provided to understand 2D materials synthesis and growth, and to interpret experimental data.

Emerging research – Future prospects

1. The development of a synergic approach among physics, photonics and material chemistry for novel applications in (photo)catalysis. (**Research areas 1, 2 and 3**).

2. A better understanding of the mechanisms involved in some selected catalytic processes (e.g. CO_2 conversion) exploring the activity of different metal centers present on catalyst surface and their interaction with molecules in gas phase. This ambitious topic will be developed taking advantage from the interaction between experimental and computational approaches. Plasmas can also be used to produce catalysts or to convert CO_2. (**Research areas 2, 3 and 4**).

STRONG POINTS

The strength of the Institute mainly stands in the tight collaboration between experts in organic and physical chemistry, materials chemistry, surface science and solid-state science from both a theoretical and experimental point of view as well as in the combination of many different preparation and characterization techniques.

1. Development of **0D, 1D, 2D and 3D** inorganic and organic/inorganic organizations, selective functionalization and applications.

2. Straightforward synthesis approaches covering the preparation of complex molecules up to nanoscale organizations passing through supramolecular assembly:

Molecular → supramolecular → nanoscale → microscopic level

3. Research and development of **outstanding characterization techniques (experimental and theoretical approaches)** including X-ray photoelectron spectroscopy, ion spectrometries, solid state nuclear magnetic resonance, vibrational and rotational spectroscopy, linear and nonlinear optical spectroscopies ….

4. Multi-scale numerical simulation approaches to predict and interpret the structures and properties of 0D, 1D, 2D, and 3D systems.

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