# PhD Thesis Subject: Optimization of Gap-plasmon Resonators

## for Environmental Systems

This PhD project is part of an interdisciplinary projet gathering experts in physics, optics, computational science and chemists. The candidate will be based between the Institut Fresnel and the IM2NP both in Marseille. At the Institut Fresnel, the candidate will work within the RCMO team experts in nanophotonics, optical nearfield microscopy and optical thin film. At the IM2NP, the candidates will work within the Lumen-PV experts in electromagnetic modelization, inverse design (ID), nanophotonics. The candidate will spend also at least two months in Germany at the HZDR in Dresden for characterization using cathodoluminescence. Furthermore, the project will benefit of the strong collaboration with the CINaM in Marseille, crucial for the fabrication of the nanoparticles-on-mirror systems.

This project was selected as AMU's SCHADOC program. This program is MSCA - COFUND doctoral program co-funded by Europe, the Région Sud and Amidex. It is made to attract PhDs with training in culture, health, AI, and climate, fostering research aligned with CIVIS and regional goals. (https://schadoc.univ-amu.fr/en/call-candidates)

### **Research Overview:**

Plasmonic nanostructures, particularly Nanoparticle-on-Mirror (NPoM) configurations, offer highly localized electromagnetic field enhancements, making them ideal for sensing applications. The NPoM configuration is a specific geometry that combines a metallic nanoparticle, typically nanocubes, and a flat metallic surface separated by a dielectric nanometer-scale gap.

This PhD project aims to develop and optimize NPoM-based plasmonic sensors by combining nanoscale characterization (s-SNOM: scattering-scanning nearfield optical microscopy and CL: cathodoluminescence) with numerical inverse design (ID) methods for optimizing and predict performances. The candidate will explore how nanoparticle size, shape, spacing, and dielectric environments influence localized surface plasmon resonances (LSPRs) first for a single subunits and then over complex architectures combining several ones.

Through this project, we expect to gain a better understanding of the coupling mechanisms, between the metal thin film substrate and the nanocubes and/or between neighboring nanocubes, within the proposed complex architecture. This should allow moving towards better optimization in terms of exaltations, confinements, but also sensitivity and selectivity toward better sensing performance.

By integrating computational simulations, global optimization algorithms and/or machine learning models, and advanced experimental techniques, this research will establish a systematic framework for designing NPoM architectures with optimized plasmonic properties for applications in environmental monitoring or chemical detection. The ultimate goal will be to develop such platform at a competitive level in the field of optical sensor and a validation step is envisioned on the detection of volatile organic components (VOC).

### Implementation strategy of the PhD program by major steps:

1. Data Collection: Gather experimental data on various NPoM configurations, including parameters like nanoparticle size, shape, material composition, different types of substrates, and the resulting sensing performance metrics (first year).

2. Data Set Completion: nanoscale experimental characterization for a full understanding of the single subunit using both s-SNOM (Institut Fresnel) and CL (HZDR, Germany) (first year).

3. Optimization of the single resonant cavity: use evolutionary optimization algorithms to improve the sensing response of the single cavity by setting the size nanocube and the spacer thickness (IM2NP) (first & second year).

4. Inverse Design of the complex NPoM: use inverse design methods (Differential Evolution and Deep Learning) to improve the sensing response of the NPoM system by adding more nanocubes in the system (second year).

5. Experimental Validation: Fabricate the AI-recommended NPoM structures (in collaboration with CINaM) and validate their performance experimentally by s-SNOM and CL. A refining step of the models with new data will be done and iterate as needed (second &third year).

6. Sensing Implementation: Sensing implementation and performance evaluations of the sensitivity and selectivity of the proposed platform (third year).

#### Candidate Profile:

We are looking for an excellent candidate with a strong background and interest in optics (nanophotonics, far and nearfield optical microscopy, optical components) and in numerical programming (Python). This project gathered both cutting-edge technologies for characterization at the nanoscale and computational techniques for optimization and inverse design problems.

The candidate should be motivated, with skills in experiment and strong taste in numerical programming, with an interest in the intersection of nanophotonics and artificial intelligence for cutting-edge sensing applications.

Others eligibility criteria imposed by the call:

- The candidate should not have been affiliated to / employed by a French institution for more than 12 months in the last 3 years
- The candidate should not have carried out research for more than 4 years since obtaining their master's degree
- Acceptance to work with us will be subjected to the ZRR (restricted area) clearance.
- Application deadline April 21<sup>st</sup>, 2025, 5pm.

Keywords: Plasmonic, Characterization, Inverse Design, Nearfield optical microscopy

**For more details** on the scientific project/program, impact and fallouts, consortium and intersectoral dimensions see: <u>https://schadoc.univ-amu.fr/en/call-candidates/climate-change-environmental-</u> challenges/ogres

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