Surface Functionalization as a Key Step for E[illegible]ing Nanodiamonds with NV Centers for Bioimaging an[illegible] Sensin[illegible]

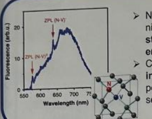
Bénédicte Malemo[1*], Anne Vallée[1], Alexi[illegible] Loiseau[1], Jean-Charles Arnault[2], Hugues Girard[2], [illegible] Boujday

[1]Laboratoire de Réa[illegible] de Surface (LRS), Sorbonne Université – France

[2]Nanosciences et Innovation pour les Matériaux, l[illegible]decine et l'Energie (NIMBE) – CEA, CNRS, Université Paris-Saclay – France

* benedicte.malemo@sorbonne-universite.fr

Introduction



- Nanodiamonds (NDs) with nitrogen-vacancy (NV) centers **are stable & biocompatible quantum emitters** (1)
- Challenge: **their fluorescence is intrinsically weak,** reducing performance in bioimaging and sensing.

Strategy

Coupling NDs to gold via **localized surface plasmon resonance (LSPR) can boost emission** (2), with expected **fluorescence increases exceeding 100-fold.**

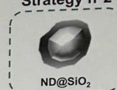
Surface functionalization

- Provide chemical versatility
- Introduce anchoring sites for gold deposition
- Control ND-Au spacing to avoid quenching of the fluorescence
- Ensure colloidal stability for bioapplications

Establishing **robust functionalization routes** to prepare NDs for **integration into plasmonic core-shell architectures** for bioimaging and sensing

Strategy n°1

Strategy n°2

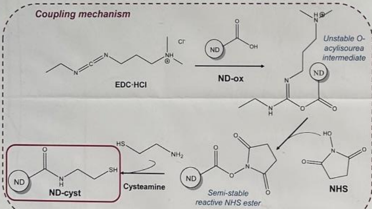


Cysteamine grafting

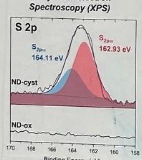
Introduce **thiol (–SH) groups** to promote affinity with **gold**

Functionalization with **cysteamine**
Activation of oxidized NDs carboxyl groups with **EDC/NHS** reaction

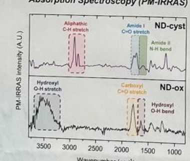
Coupling mechanism



X-Ray Photoelectron Spectroscopy (XPS)



Phase Modulation Infrared Reflection Absorption Spectroscopy (PM-IRRAS)



	C (at%)	O (at%)	N (at%)	S (at%)
ND-ox	87.7	12.1	< 0.2	0
ND-cyst	86.1	12.0	1.0	0.6

XPS data:
Increase in N content confirms cysteamine grafting
Clear **S 2p signal** detected only after functionalization → evidence of thiol groups
PM-IRRAS data consistent with successful grafting

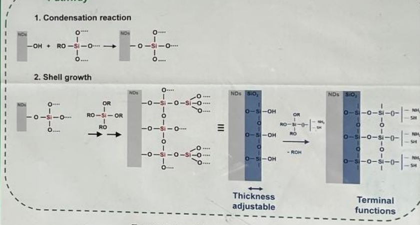
→ **Cysteamine grafting provides surface thiols as anchoring sites for future Au deposition**

Silica encapsulation

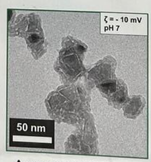
- **Control ND-gold spacing** to avoid fluorescence quenching
- **Provides chemical versatility** for easier functionalization

Sol-gel process forms tunable silica shell (SiO_2) around NDs (3)

Pathway

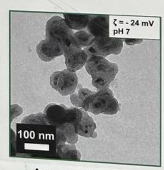


Transmission Electron Microscopy (TEM)



Average shell thickness = 5.0 ± 0.9 nm

- TEM confirms controlled silica coating, with thickness adjusted by **varying silane concentration**



Average shell thickness = 11.8 ± 2.4 nm

- Particles organize into **interconnected networks** instead of remaining individual

→ **Silica encapsulation enables control of ND-Au distance and offers a chemically versatile platform**

Conclusion

Successful surface functionalization of NDs is demonstrated through two strategies: **cysteamine grating and silica coating**

Functionalization = **key step** toward integrating NDs into **plasmonic core-shell nanocomposites**

Development of **robust functionalized platforms**

Next steps

- **Gold seed deposition & shell growth**

- **Evaluation of optical properties** (NV emission enhancement)

References:
(1) Balasubramanian, G. et al. Current Opinion in Chemical Biology 2014, 20, 69–77.
(2) Orlanducci, S. Eur J Inorg Chem 2018, 2018 (48), 5138-5145.