

# C'Nano 2020

The Nanoscience Meeting

## TOULOUSE

Centre des congrès Pierre Baudis

**POSTPONED**



**NEW  
DATES**

**November  
23, 24, 25  
2021**



### Gaël DE PAËPE

Directeur de Recherche CEA

IRIG – MEM (Univ. Grenoble Alpes – CEA)

17 Avenue des Martyrs, 38054 Grenoble

<https://nmr-dnp-grenoble.net/home/>

[gael.depaepe@cea.fr](mailto:gael.depaepe@cea.fr)

### CV/ biography

Gaël De Paëpe is currently leading the NMR-DNP group at IRIG (MEM, CEA/Univ. Grenoble Alpes). He obtained his M.Sc. and Ph.D. at ENS Lyon, France, under the supervision of Prof. L. Emsley. In 2004, he went to MIT for a postdoctoral work with Prof. R. G. Griffin. He returned to France in 2008 with an ANR Chair of Excellence to set up high-field NMR-DNP at CEA Grenoble. He received the Vold Memorial Prize (2013) and a consolidator grant funded by the European Research Council (2015). He is heading the Magnetic Resonance laboratory at IRIG-MEM since 2021. His group focuses on MAS-DNP method and technology development for applications in materials science, chemistry, and biology. More specifically, the NMR-DNP group is specialized in applications ranging from organic and inorganic NCs, energy materials to biomolecular systems (protein-ligand/ protein fibrils). The group is also a global leader in the development of new instrumentation and polarizing agents for MAS DNP at ultra-low temperature.

### Probing ligand coordination in Zinc oxide nanocrystals enabled by Dynamic Nuclear Polarization enhanced solid-state NMR

#### Abstract

ZnO nanocrystals (NCs) have attracted significant research efforts owing to their versatility, with applications in numerous fields including catalysis, semiconductors, and in paint and rubber industries, as well as for their anti-microbial activity. Their shape, size, bulk composition (including the presence of dopant/vacancy), but also the ligand capping of these NCs determine their optoelectronic properties and their suitability for a particular application. Control over these parameters is a long-standing challenge, which implies establishing and optimizing new synthetic approaches. Nevertheless, the unambiguous characterization of the coordination chemistry of NC surfaces produced by wet-chemical synthesis remains a highly challenging issue.

In this presentation, we will show that Dynamic Nuclear Polarization combined with Magic Angle Spinning (MAS-DNP) can provide enough sensitivity to probe the ligand structure through multidimensional NMR experiments, which can be used to extract unprecedented information concerning ligand arrangements on NC surfaces.<sup>1,2</sup>

First, we will highlight the vast difference between the organic-inorganic interfaces resulting from two synthetic routes to ZnO NCs capped with organophosphorous ligands: a traditional sol-gel approach and an organometallic approach called OSSOM (One-pot Self-Supporting OrganoMetallic).<sup>1</sup> MAS-DNP-enhanced NMR not only supplies a detailed NC surface analysis but also demonstrates the interest of the OSSOM approach for the preparation of highly stable quantum sized ZnO spherical nanocrystals. We will further discuss how MAS-DNP NMR can be used to determine ligand coordination modes and atomic-scale arrangements on faceted hexagonal ZnO nanoplatelets obtained through an organometallic approach.<sup>2</sup> Overall, this work relating ligand-binding modes with particle morphology will contribute to a rational design of tailored nanocrystals.

**References:** (1) D. Lee, M. Wolska-Pietkiewicz, S. Badoni, A. Grala, J. Lewiński, G. De Paëpe, *Angew. Chemie - Int. Ed.* **2019**, 58 (48), 17163–17168. (2) M. Terlecki, S. Badoni, M. K. Leszczyński, S. Gierlotka, I. Justyniak, H.

**Keywords:** ZnO nanocrystals, Dynamic Nuclear Polarization, solid-state NMR, ligand-NC interaction