Lorenzo Niccoli

Postdoctoral Researcher

ETH Zürich
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Magnetic resonance scientist with a strong programming background, focused on spin dynamics and optimal control. Experienced in solid-state NMR, DNP, ESR, and HPC systems.

Content

Professional Experience

Jan. 2025 – Present **Postdoctoral researcher**, ETH Zürich, Zürich, Switzerland.

• Optimization of pulse sequences for solid-state Nuclear Magnetic Resonance (NMR) and Dynamic Nuclear Polarization (DNP) using optimal control and Floquet theory.

• Teaching assistant for Thermodynamics for Pharmacist and Advanced Magnetic Resonance (Solid-state NMR, Relaxation). Total lecture time $>$ 130 h.

Nov. 2024 – Dec. 2024 **Postdoctoral researcher**, CIRMPP, Florence, Italy.

• Solid-State NMR on low-gamma nuclei (^{89}Y) on YAG ceramics.

• Simulation of polarization diffusion (electron-to-proton) in DNP experiments under magic angle spinning (MAS) conditions.

Education

Nov. 2021 – Nov. 2024 **Ph.D. in Chemistry** – École Normale Supérieure, Lyon, France
Ph.D. in Structural Biology – University of Florence, Florence, Italy

Supervisors: Dr. A. Lesage and Prof. M. Lelli

• Development of novel polarizing agents for DNP at high magnetic fields and fast Magic Angle Spinning (MAS) in solid-state NMR from an experimental and computational perspective.

Oct. 2019 – Sept. 2021 **M.Sc. in Chemistry** – University of Florence, Florence, Italy

Sept. 2016 – Oct. 2019 **B.Sc. in Chemistry** – University of Florence, Florence, Italy

Professional Skills

Expertise	NMR & DNP • Density Functional Theory (DFT) • Optimal Control • Electron Spin Resonance (ESR) • High-Performance Computing (HPC).
Programming	MATLAB • Python • C • FORTRAN • bash • LaTeX.
Libraries	Spinach (MATLAB) • EasySpin (MATLAB) • PLUMED (GROMACS).
Software	GROMACS • ORCA • GAUSSIAN • CP2K • TopSpin • Mathematica • Adobe Illustrator • Inkscape.
Dev Tools	Git • Docker • SLURM • PBS.
Languages	Italian (native) • English (C1) • French (B1) • German (A2)

Awards and Grants

2024	**65th Experimental NMR Conference**	Travel stipend	**$800**
2022	**Italian NMR Organization (GIDRM)**	Travel grant	**€678**
2022	**Italian-French University "Vinci Grant"**	Research grant	**€4,500**

Conference Presentations

Feb. 2026	**Swiss NMR conference**, Lausanne, Switzerland. *Oral presentation*: "DNP pulse sequence optimization with effective Hamiltonians".
Sept. 2025	**Alpine Conference on Magnetic Resonance in Solids**, Chamonix-Mont-Blanc, France. *Oral presentation*: "DNP pulse sequence engineering through Floquet effective Hamiltonians".
May 2024	**Chianti Workshop 2024**, Florence, Italy. *Poster*: "Efficient DNP at high fields and fast MAS with antenna-sensitized dinitroxides".
Apr. 2024	**Experimental NMR Conference**, Asilomar, CA, USA. *Poster*: "Tailor-designed binitroxides for DNP at high field and fast MAS".
Nov. 2023	**Second Annual PANACEA User Meeting**, Florence, Italy. **Local organizer**.
Sept. 2023	**International Hyperpolarization Conference**, Leipzig, Germany. *Oral presentation*: "Efficient dynamic nuclear polarization at high field and fast magic angle spinning from tailor-designed binitroxides".
May 2023	**4èmes Journées RMN du Grand Sud**, Lyon, France. *Poster*: "Novel polarizing agents for high-field and fast MAS DNP solid-state NMR".
Sept. 2022	**Italian-French International Conference on Magnetic Resonance**, Milan, Italy. *Poster*: "Efficient polarizing matrices for DNP MAS NMR at high magnetic fields".
Jun. 2022	**Chianti Workshop 2022**, Principina Terra, Italy. **Local organizer**. *Poster*: "A computational investigation of temperature dependence of MAS DNP NMR".

References

Prof. Matthias Ernst	ETH Zürich	maer@ethz.ch
Dr. Anne Lesage	CRMN-Lyon	anne.lesage@ens.fr
Prof. Moreno Lelli	University of Florence	moreno.lelli@unifi.it

Publications

(1) Niccoli, L.; Camenisch, G.-M.; Chávez, M.; Ernst, M. Effective Hamiltonians based DNP sequence optimization. *J. Phys. Chem. Lett.* **2026**, *17*, 3084–3090, DOI: 10.1021/acs.jpclett.5c03855.

(2) Badoni, S.; Berruyer, P.; Niccoli, L.; Lesage, A.; Emsley, L. Maximizing Relayed 1H Hyperpolarization Transfer by Slow-Fast MAS NMR Spectroscopy. *J. Phys. Chem. A* **2024**, *128*, 7005–7012, DOI: 10.1021/acs.jpca.4c02452.

(3) Niccoli, L.; Casano, G.; Menzildjian, G.; Yulikov, M.; Robinson, T.; Akrial, S.-E.; Wang, Z.; Reiter, C.; Purea, A.; Siri, D.; Venkatesh, A.; Emsley, L.; Gajan, D.; Lelli, M.; Ouari, O.; Lesage, A. Efficient DNP at high fields and fast MAS with antenna-sensitized dinitroxides. *Chem. Sci.* **2024**, *15*, 16582–16593, DOI: 10.1039/D4SC04473H.

(4) Tricomi, J.; Cacaci, M.; Biagiotti, G.; Caselli, L.; Niccoli, L.; Torelli, R.; Gabbani, A.; Vito, M. D.; Pineider, F.; Severi, M.; Sanguinetti, M.; Menna, E.; Lelli, M.; Berti, D.; Cicchi, S.; Bugli, F.; Richichi, B. Ball milled glyco-graphene oxide conjugates markedly disrupted Pseudomonas aeruginosa biofilms. *Nanoscale* **2022**, *14*, 10190–10199, DOI: 10.1039/D2NR02027K.

(5) Menzildjian, G.; Lund, A.; Yulikov, M.; Gajan, D.; Niccoli, L.; Karthikeyan, G.; Casano, G.; Jeschke, G.; Ouari, O.; Lelli, M.; Lesage, A. Efficient Dynamic Nuclear Polarization up to 230 K with Hybrid BDPA-Nitroxide Radicals at a High Magnetic Field. *J. Phys. Chem. B* **2021**, *125*, 13329–13338, DOI: 10.1021/acs.jpcb.1c07307.

In Preparation

– Niccoli, L. et al. Optimization of DNP sequences with Floquet Effective Hamiltonians.