

# Computational methods and NMR spectroscopy: a powerful synergy for chemistry, materials science and biology

10<sup>th</sup> December 2019

Pisa "Le Benedettine" conference center

Gathering contributes from experts in the fields, the aim of the workshop is to present the great potential of combining NMR spectroscopy and computational methods for structural elucidations of small molecules, proteins and materials, both in liquid and solid phases. The meeting is intended as an opportunity for a broad audience of interested researchers, from academy and industry, working in materials science and technology, chemistry and life sciences.

## Scientific Program

09.30 Registration  
10.15 Opening

10.30 **Benedetta Mennucci** (University of Pisa)  
The simulation of spectroscopies of biological systems: a multiscale approach

11.00 **Alexandre M.J.J. Bonvin** (Utrecht University)  
Integrative modelling of biomolecular complexes

11.30 **Antonio Rosato** (University of Firenze)  
Evolutionary constraints in NMR-based protein structure determination

12.00 **Giacomo Saielli** (CNR-ITM, Padova)  
DFT-NMR for structure elucidation: from single molecules to bulk ionic liquids

12.30 Lunch

14.00 **Davide Ceresoli** (CNR-ISTM, Milano)  
DFT calculation of NMR parameters with the GIPAW method

14.30 **Michele Chierotti** (University of Torino)  
NMR crystallography in crystal engineering: what's inside our computational and NMR toolboxes

15.00 **Alfonso Pedone** (University of Modena and Reggio Emilia)  
Computational NMR spectroscopy as a new tool to probe materials structures

15.30 **Thibault Charpentier** (CEA Paris-Saclay)  
Combining experimental and computational solid state NMR for structure determination of oxide glasses

16.00 Closing

### Scientific Committee

S. Borsacchi, L. Calucci, E. Carignani,  
M. R. Chierotti, M. D'Onofrio,  
M. Geppi, F. Martini, G. Pileio, P. Turano

### Organizing Committee

Silvia Borsacchi (CNR-ICCOM)  
Elisa Carignani (UNUPI-DCCI)  
Francesca Martini (UNUPI-DCCI)

 [pisa2019@gidrm.org](mailto:pisa2019@gidrm.org)

### Information

Register at [www.gidrm.org](http://www.gidrm.org)  
Deadline: **30<sup>th</sup> November**  
Registration Fees:  
50 € for non GIDRM members  
30 € for 2019 GIDRM members



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