

# **COMPUTATION OF NMR PROPERTIES**

*13<sup>th</sup>-17<sup>th</sup> November 2017*

*CEA-INSTN*

*[www-instn.cea.fr/en/](http://www-instn.cea.fr/en/)*

*Chair “Materials Simulation & Engineering”*

*[www.chair-mse.org](http://www.chair-mse.org)*

*Maison de la Simulation*

*[www.maisondelasimulation.fr/en/](http://www.maisondelasimulation.fr/en/)*

*CEA Saclay, France*

# Monday

- 08:45 - 09:00 **Welcome**  
C. Meis (INSTN-CEA) and T. Charpentier (DRF-CEA)
- 09:00 - 09:50 **Physics of NMR**  
M.H. Levitt, University of Southampton, U.K.
- 09:50 - 10:00 Discussion-Questions
- 10:00 - 10:30 Coffee break
- 10:30 - 11:20 **NMR interactions**  
M.H. Levitt, University of Southampton, U.K.
- 11:20 - 11:30 Discussion-Questions
- 11:30 – 12:20 **NMR spectroscopy**  
N.Giraud, Université Paris Saclay – UPSUD, France
- 12:20 – 12:30 Discussion-Questions
- 12:30 - 14:00 Lunch
- 14:00 – 14:45 **Introduction to NMR simulations techniques**  
J.N. Dumez, CNRS, Gif-sur-Yvette, France
- 14:45 – 17:15 **Computer Session – Spin dynamics and NMR spectral simulations**  
J.N. Dumez, CNRS, Gif-sur-Yvette, France  
C. Martineau, Université Paris Saclay – UVSQ, France  
T. Charpentier, CEA – Saclay, France  
N. Giraud, Université Paris-Sud – UPSUD, France

# Tuesday

- 09:00 – 09:40 *First-principles, DFT (I)*  
*J.D. Gale, Curtin University, Australia*
- 09:40 – 09:45 *Discussion-Questions*
- 09:45 – 10:25 *First-principles, DFT (II)*  
*J.D. Gale, Curtin University, Australia*
- 10:25 – 10:30 *Discussion-Questions*
- 10:30 – 10:50 *Coffee break*
- 10:50 – 11:30 *Quantum chemistry for NMR of molecular systems (I)*  
*A.A. Auer, Max Planck Institute, Germany*
- 11:30 – 11:35 *Discussion-Questions*
- 11:35 – 12:15 *Quantum chemistry for NMR of molecular systems (II)*  
*A.A. Auer, Max Planck Institute, Germany*
- 12:15 – 12:20 *Discussion-Questions*
- 12:30 – 14:00 *Lunch*
- 14:00 – 17:00 *Computer Session – Computation of NMR parameters with localized basis-sets. (ORCA)*  
*A. A. Auer, Max Planck Institute, Germany*  
*J.P. Dognon and T. Charpentier, CEA –Saclay, France*

# Wednesday

- 09:00 – 09:40 *DFT-GIPAW - NMR parameters using plane wave DFT (I)*  
*A. Seitsonen, ENS ULM, Chemistry Department, France*
- 09:40 – 09:50 *Discussion-Questions*
- 09:45 – 10:25 *DFT-GIPAW - NMR parameters using plane wave DFT (II)*  
*A. Seitsonen, ENS ULM, Chemistry Department, France*
- 10:25 – 10:30 *Discussion-Questions*
- 10:30 – 10:50 *Coffee break*
- 10:50 – 11:30 *GIPAW in NMR crystallography*  
*C. Martineau, Université Paris Saclay – UVSQ, France*
- 11:30 – 11:35 *Discussion-Questions*
- 11:35 – 12:15 *GIPAW in NMR of quadrupolar nuclei*  
*F. Fayon, CNRS, CEMTHI, France*
- 12:15 – 12:20 *Discussion-Questions*
- 12:30 – 14:00 *Lunch*
- 14:00 – 17:00 *Computer Session – Computation of NMR parameters using the DFT-GIPAW method.*  
*A. Seitsonen, ENS ULM, Chemistry Department, France*  
*T. Charpentier, CEA – Saclay, France*  
*C. Martineau, Université Paris Saclay – UVSQ, France*  
*F. Fayon, CNRS, CEMTHI, France*

# Thursday

- 09:00 – 09:40 **Molecular dynamics**  
*M. Salanne, PHENIX, Paris VI, France*
- 09:40 – 09:45 *Discussion-Questions*
- 09:45 – 10:25 **Disordered solids**  
*J.V. Hanna, University of Warwick, Physics Department, U.K.*
- 10:25 – 10:30 *Discussion-Questions*
- 10:30 – 10:50 *Coffee break*
- 10:50 – 11:30 **Ab initio simulations for MRI**  
*R. Pollet, CEA- Saclay, France*
- 11:30 – 11:35 *Discussion-Questions*
- 11:35 – 12:15 **Amorphous solids and glasses**  
*T. Charpentier, CEA – Saclay, France*
- 12:15 – 12:20 *Discussion-Questions*
- 12:30 – 14:00 *Lunch*
- 14:00 – 17:00 **Computer Session: disordered systems**  
*C. Martineau, Université Paris Saclay – UVSQ, France*  
*F. Fayon, CNRS, CEMTHI, France*  
*A. Seitsonen, ENS France*  
*T. Charpentier, CEA – Saclay, France*

# Friday

- 09:00 – 10:00 *Perspectives in solids / GIPAW*  
*J.V. Hanna (U.K), University of Warwick, U.K*
- 10:00 – 10:10 *Discussion-Questions*
- 10:10 – 10:30 *Perspectives in molecular systems*  
*J.D. Gale, Curtin University, Australia*
- 10:30 – 10:40 *Discussion-Questions*
- 10:40 – 11:00 *Coffee break*
- 11:00 – 12:00 *Feedback / Conclusions*
- 12:30 – 14:00 *Lunch*

***End of the School***