" Computation of NMR properties "

INSTN CEA Saclay, November 13-17, 2017

➢ An introduction to NMR physics	**M.H. LEVITT,** University of Southampton, U.K.
➢ Principles of NMR spectroscopy in liquids and solids	**M.H. LEVITT,** University of Southampton, U.K.
➢ NMR interactions – NMR parameters	**N. GIRAUD,** University Paris-Saclay, UPSUD, France
➢ Principles of NMR simulations	**J.N. DUMEZ,** CNRS, Gif-sur-Yvette, France
➢ First-principles, Density Functional Theory (DFT)	**J.D. GALE,** Curtin University, Australia
➢ Quantum chemistry for NMR of molecular systems	**A. AUER,** Max Planck Institute, Germany
➢ DFT-GIPAW: NMR parameters using plane wave DFT	**A. P. SEITSONEN,** ENS France
➢ GIPAW in NMR crystallography	**C. MARTINEAU,** University Paris-Saclay, UVSQ, France
➢ GIPAW, NMR of quadrupolar nuclei	**F. FAYON,** CNRS, CEMTHI, France
➢ Molecular dynamics	**M. SALANNE,** Maison de la Simulation, France
➢ Disordered solids	**J.V. HANNA**, University of Warwick, U.K.
➢ Ab-initio simulations for MRI	**R. POLLET,** CEA – IRAMIS, Saclay, France
➢ Amorphous solids - Glasses	**T. CHARPENTIER,** CEA – IRAMIS, Saclay, France
➢ Perspectives in solids, GIPAW methods	**J.V. HANNA,** University of Warwick, U.K.
➢ Perspectives in molecular systems	**J.D. GALE,** Curtin University, Australia

Computer sessions using relevant software:

➢ Simulation of NMR spectra	**J.N. DUMEZ**, **C. MARTINEAU, T. CHARPENTIER & N. GIRAUD**
➢ Computation of NMR parameters – Molecular systems	**J.P. DOGNON, T. CHARPENTIER & A. AUER**
➢ Computation of NMR parameters – DFT GIPAW	**A.P. SEITSONEN, T. CHARPENTIER, C. MARTINEAU & F. FAYON**
➢ Disorderd systems	**A.P. SEITSONEN, T. CHARPENTIER, C. MARTINEAU & F. FAYON**

Organizers:

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Jean-Pierre DOGNON, CEA - IRAMIS, Saclay
Charlotte MARTINEAU, University Paris-Saclay, UVSQ
Jean-Nicolas DUMEZ, CNRS
Constantin MEIS, CEA - INSTN, Saclay

Registration deadline: October 16, 2017

On-line Registration: www.mse-chair.org

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