Report on GIPAW-NMR tutorial, September 21st–24th in Zurich

We organised a tutorial on the GIPAW-NMR method. The purpose of the tutorial was to introduce the first-principles computation of Nuclear Magnetic Resonance (NMR) parameters to participants from both the experimental and computational communities.

NMR is a powerful technique in many disciplines, and now widely used for the structural characterization of a broad class of materials. However, correlating the observed spectra with the structure often requires numerical modelling to unequivocally identify all the observed resonances. A theoretical method based on the explicit solution of the electronic structure is the most reliable and predictive approach for the NMR parameters. One of the most successful and numerically feasible methods for ab initio calculation is density functional theory (DFT). Whereas there have long been approaches available in the literature to calculate NMR parameters in finite samples (molecules and clusters), for many years it was not possible to compute all the relevant parameters in the condensed phase (i.e. periodic solids). Traditionally plane wave basis has been used in conjunction with pseduo-potentials in solid-state DFT codes. There the Coulombic interaction between the ionic cores and the electrons is replaced by an effective *pseudo potential* that usually includes a non-local term in the angular channel. The Gauge Including Projector Augmented Waves (GIPAW) ["All-electron magnetic response with pseudopotentials: NMR chemical shifts", Chris J Pickard and Francesco Mauri, Phys. Rev. B **63** (2001) 245101; doi:10.1103/PhysRevB.63.245101] provided a route to computing NMR parameters in solids with all-electron accuracy. The results in "normal" materials are of nearly or practically the same level of accuracy as the all-electron methods in finite system. As implementations of the GIPAW method have in recent years achieved a level of robustness by which they can play a key role alongside experimental NMR studies, we organised this tutorial in order to allow a wider community to take advantage of these codes in their research.

The tutorial was structured so that both experimentalists (with little or no knowledge of DFT) and theorists (with little knowledge of practical NMR spectroscopy) could attend, and therefore plenary presentations on both aspects were included at the beginning of the tutorial. More detailed topics were lectured in the mornings, and in the afternoons practical terminal sessions were conducted. The two first days were devoted to establishing the basics of both NMR spectroscopy and DFT as applied to the calculation of NMR parameters. During the third and fourth days applications of GIPAW-NMR calculations in both organic and inorganic materials were presented. Advanced features of DFT calculations were also described and we elected to give a short introduction to the computation of vibrational parameters, as there is a great interest in the NMR community in understanding the effect of thermal motion on NMR parameters.

We used the DFT-GIPAW package implemented in the code PWSCF in the Quantum Espresso (QE) package (http://www.quantum-espresso.org/). There were also six contributed talks by participants, illustrating the state of the art in the application of solid-state NMR into real scientific problems and materials. After the tutorial the participants are expected to be sufficiently familiar with the GIPAW-NMR method to the extent that they can start new projects, with possibly the support from colleagues or following discussion on open forums dedicated to such topics.

There were 25 participants from across 10 European countries, and one participant each from India and Japan.

After the tutorial we arranged an anonymous survey to let the participants give feedback about the event, and seven persons made the survey. The major indicator was the "usefulness

of the tutorial", where the evaluation was done on scale from "1" (not useful at all) to "10" (very useful): The average rating was 8.57, with all the responses were from "7" to "10". Of the responses six stated that they were determined to use the GIPAW-NMR methodology in the future in their research, and the seventh one was also considering it. Thus we conclude that the tutorial filled its purpose, and we look forward for further applications appearing as a result of the tutorial.

We acknowledge the financial support for the tutorial from CECAM (http://www.cecam.org/), psi-k network (http://www.psi-k.org/), RMN structurale dans le Bassin Parisien (France) (http://rmngbp.cnrs-orleans.fr/) and CCP9 (UK) (http://www.ccp9.ac.uk).

Ari P Seitsonen *(CNRS-IMPMC and Pierre and Marie Curie University, Paris 6; University of Zurich)*
Jonathan Yates *(Oxford University)*
Thibault Charpentier *(French Atomic Energy Commission (CEA), Saclay)*

Program

Monday

- 9:45 - 10:30 Principles of NMR (ThC)
- 10:30 - 11:00 Coffee
- 11:00 - 12:30 DFT in the solid-state (APS)
- 12:30 - 14:00 Lunch break
- 14:00 - 18:00 Practical Session: Introduction to the usage of the QE package and application to basic DFT calculations (convergence, energy cut-off, K-grid, etc)

Tuesday

- 9:00 - 10:00 Calculation of NMR Parameters (JRY)
- 10:00 - 10:30 Coffee
- 10:30 - 11:30 Advanced NMR (ThC)
- 11:30 - 13:30 Lunch break
- 13:30 - 14:00 Geometry and Dynamics (JRY)
- 14:00 - 18:00 Practical Session: Usage of the GIPAW-NMR software

Wednesday

- 9:00 - 9:30 Applications to Inorganic (ThC)
- 9:30 - 10:30 Vibrational Spectroscopy (PG)
- 10:30 - 11:00 Coffee
- 11:00 - 11:30 Applications to Organic Materials (JRY)
- 11:30 - 12:30 Participant Presentations
    - John Hanna
    - Nicolas Foliet
    - Giacomo Saielli
- 12:45 - 14:00 Lunch break
- 14:00 - 18:00 Practical Session: Relaxation of structures in conjunction with NMR calculations

Thursday

- 9:00 - 9:30 Introduction to QE (PG)
- 9:30 - 10:15 Advanced DFT (APS)
- 10:15 - 10:45 Coffee
- 10:45 - 11:30 Pseudopotentials (PG)
- 11:30 - 12:30 Participant Presentations
    - Simona Ispas
    - Filipe Vasconcelos
    - Sylvian Cadars
- 12:30 - 14:00 Lunch break
- 14:00 - 18:00 Practical Session: Vibrational calculations, NMR parameters under pressure and participant's own examples

Participants

- Organisers and lecturers
    - Thibault CHARPENTIER France, French Atomic Energy Commission (CEA)
    - Ari Paavo SEITSONEN France, CNRS and Université Pierre and Marie Curie
    - Jonathan YATES United Kingdom, Oxford University
    - Paolo GIANNOZZI Italy, Università di Udine, Dipartimento di Fisica
    - Layla MARTIN-SAMOS Italy, CNR-INFM S3
- Participants
    - Emmanuel BETRANHANDY France, Ecole Polytechnique
    - Goranka BILALBEGOVIC Croatia, University of Zagreb, Department of Physics
    - Monique BODY France, Université de Maine, LEPC CNRS UMR 6087
    - Sylvian CADARS France, CNRS, CEMHTI
    - Minseok CHOI Japan, University of Kyoto, Department of Materials Science and Engineering
    - Laurent DELEVOYE France, UCCS
    - Franck FAYON France, CNRS, CEMHTI
    - Guillaume FERLAT France, IMPMC, Université Pierre et Marie Curie Paris VI
    - Christian FERNANDEZ France, Université de Caen, CNRS, ENSICAEN
    - Xenia FILIP Romania, National Institute for Research and Development of Isotopic and Molecular Technologies
    - Calin Gabriel FLOARE Romania, National Institute for Research and Development of Isotopic and Molecular Technologies
    - Nicolas FOLLIET France, Laboratoire de Chimie de la Matière Condensée de Paris
    - John HANNA United Kingdom, University of Warwick, Department of Physics
    - Simona ISPAS France, Université Montpellier II, LCVN
    - Robert LASKOWSKI Austria, Vienna University of Technology
    - Luis MAFRA Portugal, Aveiro, Department of Chemistry
    - Gregor MALI Slovenia, National Institute of Chemistry
    - Carlo NERVI Italy, University of Turin, Department of Chemistry IFM
    - Geo PAUL Italy, Università del Piemonte Orientale
    - Ali Hussain RESHAK Czech Republic, South Bohemia University
    - Giacomo SAIELLI Italy, CNR Institute on Membrane Techonology
    - Neeraj SINHA India, Centre of Biomedical Magnetic Resonance
    - Iurii TIMROV France, Ecole Polytechnique

- Filipe VASCONCELOS France, Université des Sciences et Technologies de Lille, UCCS, Unité de Catalyse et de Chimie du Solide
- Aurélie VICENTE France, Université de Caen, Laboratoire Catalyse et Spectrochimie

Psi-k Network : Towards Atomistic Materials Design

Psi-k
Daresbury Science & Innovation Campus
Daresbury, Warrington
WA4 4AD
UK

Tel: +44 (0)1925 603227
Fax: +44 (0)1925 603634

PSI-K TUTORIAL FINANCE REPORT

Title of the Tutorial	Calculation of Solid-State NMR Parameters Using the GIPAW Methods
Tutorial Organisers	Thibault Charpentier / Ari Paavo Seitsonen / Jonathan Yates
Location of the Tutorial	ETH-Zurcih, Switzerland
Dates of the Tutorial	September 21st to September 24th, 2009
Total Grant from Psi-k	2 200 €

EXPENDITURE

(Please complete the tables using numbers ONLY in the amounts fields - the spreadsheet will calculate the totals for y

WORKSHOP DELEGATES / SPEAKERS			
Name and Country of Claimant	**Travel**	**Accommodation**	**Total (€'s)**
SAIELLI Giacomo	276.31 €		€ 276.31
FILIP Xenia	194.50 €		€ 194.50
RESHAK Ali Hussain	377.23		€ 377.23
SINAH Neeraj	535.33 €		€ 535.33
SEITSONEN Ari Paavo	€ 298.00		€ 298.00
MARTIN SAMOS Layla		€ 400.00	€ 400.00
LASKOWSKI Robert		€ 300.00	€ 300.00
			€ -
			€ -
			€ 2'381.37

WORKSHOP REFRESHMENTS / CONFERENCE DINNERS			
Date	**Tea / Coffee**	**Lunch / Dinner**	**Total (€'s)**
			€ -
			€ -
			€ -
			€ -
			€ -
			€ -

MISCELLANEOUS EXPENDITURE	
Details	**Total (€'s)**
	€ -

	€ 2'381.37
	€ -
	€ -

	€ 2'381.37

EMILIE BERNARD

CECAM - EPFL
PPH 338 (Bât. PPH)
Station 13
1015 Lausanne