Inmaculada Peral

Position:	Disk Chopper Spectrometer instrument scientist
E-mail:	inma@nist.gov
Phone:	+ 1 (301) 975 6235
Fax:	+ 1 (301) 921 9847
Mailing address:	Inmaculada Peral Bldg 235, Room E137 NIST Center for Neutron Research 100 Bureau Drive, Mail Stop 8562 Gaithersburg, MD 20899-8562
Date of birth:	12/08/1973

EDUCATION

Ph.D. at Universidad del País Vasco, Spain, 2001

Advisor:	Prof. G. Madariaga
Title:	Structure and orientational states in co-elastic systems: urea-inclusion compounds and the ABX_3 family
Area:	Experimental Solid-State Physics

M.A. equivalent – Physics, Universidad del País Vasco, Spain, 1997

Advisor:	Prof. G. Madariaga
M.A. thesis:	Study and modeling of the diffraction diagrams of the compound $(CH_3)_4NCdCl_3$
Area:	Experimental Solid-State Physics

B.A. equivalent – Physics, Universidad del País Vasco, 1996

Area:	Solid-State/Fundamental Physics

AWARDS

Universidad del País Vasco Predoctoral Grant, 1996/1997
Basque Regional Government Predoctoral Grant, 1997/2000
Spanish Ministry of Education Predoctoral Exchange Grant, 8-10/1997
Attended **Hercules 2000** (Higher European Research Course for Users of Large Experimental Systems), February-April 2000, Grenoble (France)

OVERVIEW OF RESEARCH ACTIVITIES

- I try to understand the guest–host intermolecular interactions in clathrate hydrates by studying their structure and vibrational spectrum

- I am combining neutron diffraction and first-principles methods to study the chemical environment of oxygen atoms diluted in titanium-rich alloys (Ti-Al in particular).

- I am investigating the local structure of zeolites using a PDF (Pair Distribution Function) approach that allows to study complicated disordered systems at intermediate length scale s ($\approx$10 $\AA$).

- I have completed a number of works in the field of non-conventional crystallography. Examples are the study of twinned, incommensurate and co-elastic systems using neutron and X-ray diffraction.

- I have studied the ferroelastic phase transitions, as well as the ferroelastic domain structure, of a number of systems such as urea inclusion compounds, members of the ABX3 family, etc.

RESEARCH EXPERIENCE

10/96-02/01	Graduate Student Universidad del País Vasco, Spain.
03/01-06/02	Post-doctoral fellow at the Chemical Engineering Department working with Raul Lobo University of Delaware, Newark DE (USA)
07/02-present	Disk Chopper Spectrometer Instrument scientist NIST Center for Neutron Research Gaithersburg MD (USA)

RESEARCH EXCHANGES

08-10/97	Research Assistant (Working on protein crystallography and protein crystallization) Departamento de Física Universidad Nacional de Colombia Bogota, Colombia.
04/00	Fakultat fur Physik und Geowissenschaften (Work on Ph.D. thesis. Acquired NMR skills) Universitat Leipzig Leipzig, Germany.

TEACHING EXPERIENCE

1997-1998	Teaching Assistant (Experimental methods in Solid State Physics) Departamento de Física de la Materia Condensada Universidad del País Vasco

LIST OF SCIENTIFIC PUBLICATIONS

[14] Structure and Dynamics of Propylene Oxide and Trimethylene Oxide Clathrate Hydrates
Proceedings of the Materials Researcg Society 2004 Fall Meeting: Neutron and X-Ray Scattering as Probes of Multiscale Phenomena. Volume 840, Editors: S.R. Bhatia, P.G. Khalifah, D. Pochan, P. Radaelli (in press)

[13] Translational dynamics of water in a nanoporous layered silicate
S. Nair, Z. Chowdhuri, I. Peral, D.A. Neumann, L.C. Dickinson, G. Tompsett, H.-K. Jeong and M. Tsapatsis
Phys. Rev. B (in press)

[12] Signature of Concentration Fluctuations in Miscible Polymer Blends from QENS
V. García-Sakai, J.K. Maranas, I. Peral and J.R.D. Copley
J. Polymer Science, Part B: Polymer Physics (submitted)

[11] Protein and Solvent Dynamics: How Strongly Are The y Coupled?
G. Caliskan, D. Mechtani, S. Azzam, J.H. Roh, A. Kisliuk, M.T. Cicerone, S. Lin-Gibson, I. Peral and A.P. Sokolov
J. Chem. Phys. 121, 1978-1983 (2004)

[10] A pair Distribution Function Analysis of Zeolite Be ta
M.M. Martinez-Inesta, I. Peral and R.F. Lobo
Microporous and Mesoporous Materials 77, 55-66 (2005)

[9] Structural Comparison of Two EUO-type Zeolites Inves tigated by Neutron Diffraction
I. Peral, C.Y. Jones, S.P. Varkey and R.F. Lobo
Microporous and Mesoporous Materials 71, 125-133 (2004)

[8] Dynamics of Trimethylene Oxide in a Structure II Cla thrate Hydrate
C.Y. Jones and I. Peral
American Mineralogist 89, 1176-1182 (2004)

[7] Structural Study of the Low Temperature Phase of TlH_2PO_4 at 180 K

E. Alvarez, G. Madariaga, I. Peral, C.L. Folcia and S. Rios
Acta Cryst. B 58, 750-759 (2002)

[6] Average Structure of the Composite Crystal Urea/Octanedioic Acid at Room Temperature within the Superspace Formalism
I. Peral, G. Madariaga, V. Petriceck and T. Breczewski
Acta Cryst. B 57, 386-393 (2001)

[5] Superspace Description of the Structure of the Urea/ n-Octane Inclusion Compound at Room Temperature
I. Peral, G. Madariaga, V. Petriceck and T. Breczewski
Acta Cryst. B 57, 378-385 (2001)

[4] Ferroelastic domain structure of $(CH_3)_4N$ C dCl_3 (TMCC) crystal
T. Breczewski, I. Peral, G. Madariaga
The European Physical Journal B, 19, 171-176 (2001)

[3] **Superspace description of the structure of the suber ic acid+urea inclusion compound at room temperature**
I. Peral, G. Madariaga, V. Petriceck and T. Breczewski
Ferroelectrics, 250, 27-30 (2001)

[2] 35Cl-NMR studies of the domain structure of tetramet hylammonium cadmium chloride (TMCC) at lower temperatures
S. Mulla-Osman, D. Michel, G. Volkel, I. Peral and G. Madariaga
J. Phys.: Condensed Matter 13, 1119-1131 (2001)

[1] X-ray diffraction study of the phase transitions of $(CH_3)_4N$ $CdCl_3$ between 293 and 80K: A quantitative analysis of th e ferroelastic domains distribution below 118K
I. Peral, G. Madariaga, A. Pérez-Etxebarria and T. Breczewski
Acta Cryst. B 56,215-225 (2000)

SCIENTIFIC EXPERIMENTAL SKILLS

Instruments and Large Facilities

- Broad knowledge of DCS, Disk Chopper Spectrometer at the NIST Center for Neutron Research, Gaithersburg MD, USA.

- Working knowledge of the four-circle Enraf-Nonius **CAD4 diffractometer**, the **STOE IPDS** using monochromated Mo-K_α radiation (on single crystal samples), the **STOE** focusing beam transmission diffractometer equipped with a linear position sensitive detector using monochromatic Cu-$K_{\alpha 1}$ radiation (on powder samples).

- Broad knowledge of the classical X-ray diffraction photographic techniques based on single crystal samples: precession camera and Weissenberg camera (using filtered Mo-K_α and Cu-K_α radiation).

- Experience performing low-temperature measurements with cryostats, close cycle refrigerators and nitrogen-gas-flow cooling systems.

- Experience performing Time-of-flight measurements at neutron sources:

  * **GLAD** and **SEPD-IPNS** (Intense Pulsed Neutron Source), Argonne National Lab. (Chicago, IL, USA)

  * **HIPPO** and **NPD- LANSCE** (Los Alamos Neutron Science Center), Los Alamos National Laboratory, (Los Alamos, NM, USA)

- Experience performing powder diffraction at neutron sources:

  * **BT1- NCNR** (NIST Center for neutron research), Gaithersburg, MD, USA

  * **3T2- LLB** (Laboratoire Leon Brillouin), Saclay, France

- Experience performing Prompt Gamma Activation Analysis on **NG7-NCNR** (NIST Center for Neutron Research), Gaithersburg, MD, USA.

- Attended hands-on tutorial courses on neutron and synchrotron radiation at the **ESRF** (European Synchrotron Radiation Facility), **CEA** (Comisariat a la Energie Atomique), **ILL** (Institut Laue-Langevin), and the **LLB** (Laboratoire Leon Brillouin):

  * Small angle scattering (**D22-ILL**)

  * Topography (**ID19-ESRF**)

* Triple-axis spectrometry (**IN3-ILL** and **LLB**)
* Powder diffraction (**DIB-ILL** and **LLB**)
* Time-of-flight (**IN6-ILL**)
* Small angle scattering (**CEA**)
* Diffuse scattering (**BM2-ESRF**)

COMPUTING EXPERIENCE

Platforms:	UNIX, Linux and VMS workstations, PC under Windows 95/98/NT/00/XP, Macintosh under MacOS 8
Software:	Structure refinement for small molecules and zeolites (EXPO, SIR, JANA,SHELXL, XTAL, FULLPROF, GSAS) Diffraction diagrams moleling and refinement (Discus, Diffax) First principles Calculations (newcomer) (ABINIT, SIESTA and CASTEP) Structural display (Cerius2, Ortep and Gretep) Document typesetting (LaTeX, Microsoft Word) Presentation (Microsoft PowerPoint, Adobe Illustrator) Graphics and image (Adobe Photoshop, xv, xfig) Data analysis (Mathematica, Origin and Kaleidagraph) Languages (Fortran, IDL, HTML and basic knowledge of perl)

ATTENDED CONFERENCES

DISMOS6: Garchy (France), May 30th - June 3th

Talk: 'Structure of urea suberic acid inclusion compound at room temperature and below 205K'

Poster: 'Unusual features in the X-ray diffraction diagrams of N(CH3)4CdCl3 between 298 K and 80K'.

IUCR99: Glasgow (UK), August 4th - 11th, 1999

Poster: 'Structure of urea suberic acid inclusion compound at room temperature and below 205K'

Aperiodic2000: Nijmegen (The Netherlands), June 4th-9th, 2000

Talk: 'Superspace description of the structure of the suberic acid+urea inclusion compound at room temperature'

ECM19: Nancy (France), August 26th - 31th, 2000

Poster: 'Structure of the octane+urea inclusion compound at 293 K'

ACA2001: Los Angeles, CA (USA), July 21st - July 26th, 2001

Workshop "From Semiconductors to proteins: Beyond the average structure"
Traverce City, MI (USA), July 28th- August 1st, 2001

NECZA2001: North East Corridor Zeolite Association, December 7th, 2002

Poster: Local Structure of Zeolite Beta from Neutron Scattering Data

Scientific Opportunities for Cold Neutron Spectroscopy Workshop, July 14th - 16th, 2003

NECZA2003: North East Corridor Zeolite Association, December 12th, 2003

Poster: 'Structural Comparison of Two EUO-type Zeolites Investigated by Neutron Diffraction'

REFERENCES

Dr. John R.D. Copley
Instrument Responsible
National Institute of Standards and Technology
100 Bureau Drive, Stop 8562
Gaithersburg, MD 20899-8562 (UNITED STATES)
Phone: +1 301 975 5133 (office), +1 301 975 6220 (secretary)
Fax:+1 301 921 9847
E-mail:john.copley@nist.gov

Dr. Raul F. Lobo
Associate Professor of Chemical Engineering
Department of Chemical Engineering
Center for Catalytic Science and Technology
University of Delaware
Newark, Delaware 19716 (UNITED STATES)
Phone: +1 302 831 1261
Fax: +1 302 831 2085
E-mail: lobo@che.udel.edu, lobocabezas@earthlink.net

Dr. Vaclav Petricek
Institute of Physics
Academy of Sciences of the Czech Republic
Na Slovance 2
182 21 Prague 8 (CZECH REPUBLIC)
Phone: (420-2) 66 05 11 11
E-mail: petricek@fzu.cz

Prof. Juan Manuel Pérez-Mato
Departamento de Física de la Materia Condensada
Facultad de Ciencias
Universidad del País Vasco
Apartado 644, 48080 Bilbao (SPAIN)
Phone: +34 94 601 2000
Fax: +34 94 464 8500
E-mail: wmppemam@lg.ehu.es

Prof. Gotzon Madariaga
Departamento de Física de la Materia Condensada
Facultad de Ciencias
Universidad del País Vasco
Apartado 644, 48080 Bilbao (SPAIN)
Phone: +34 94 601 2467
Fax: +34 94 464 8500
E-mail: wmpmameg@lg.ehu.es

Prof. Alberto García
Departamento de Física de la Materia Condensada
Facultad de Ciencias
Univesidad del País Vasco
Apartado 644, 48080 Bilbao (SPAIN)
Phone: +34 94 601 5324
Fax: +34 94 464 8500
E-mail: wdpgaara@lg.ehu.es