

## CURRICULUM VITAE SUMMARY (July, 2006):



**NAME:** RODRIGUEZ-CARVAJAL Juan  
**DATE OF BIRTH:** July 7, 1953.  
**PLACE OF BIRTH:** Sevilla, Spain.  
**NATIONALITY:** Spanish  
**MARITAL STATUS:** Married, one son.  
**QUALIFICATION:** Doctor in Physics (Solid State),  
University of Barcelona 1984.  
**PRESENT POSITION:** Diffraction Group Leader at ILL  
**LANGUAGES:** Spanish, French and English.

- **Research and Teaching** experience in Condensed Matter Physics and Crystallography for twenty six years.
- **Specialised in:**
  - Powder and single crystal x-rays and neutron scattering.
  - Symmetry analysis, crystallography and magnetism.
  - Oxides presenting remarkable properties: superconductivity,  
giant magnetoresistance,  
charge, spin & orbital ordering.
  - Computer programming and data analysis.
  - Neutron diffraction instrumentation.
- **Publications:** 198 regular papers in journals, 102 papers in journals resulting from proceedings, 58 reports/book/proceedings contributions and about 220 communications in meetings. The total number of article citations is 5293; and other citations (reports) is 2488
- **Supervisor** of 8 doctoral theses, 18 stages and post-docs.
- **Invited** to more than 60 international events (courses and conferences).
- **Author** of FULLPROF, one of the most used powder diffraction computer programs in the world. (1511 citations of the article Physica B **192**, 55 (1993) plus more than 2170 direct citations of the use of the program)
- **Working** at the Institut Laue-Langevin as Diffraction Group Leader, <http://www.ill.fr>.

## PROFESSIONAL POSITIONS HELD

1. Teaching positions in different universities (Universidad de Tarragona, Universidad de Barcelona, Universidad Politécnica de Barcelona) and temporary research positions at Laboratoire de Cristallographie in Grenoble from 1979 to 1986.
2. "Investigador Científico" at the Consejo Superior de Investigaciones Científicas. Instituto de Ciencia de Materiales de Barcelona (February 1986 to January 1988).
3. Physicist at the I.L.L. since February 1988 to 31 June 1994. Co-responsible of D4 until April 1991 and afterward co-responsible of D9. College 5B secretary ("Crystal Physics and Magnetism") from June 1990 to July 1992.
4. "Colaborateur Temporaire Etranger" at the Commissariat à l'Energie Atomique (CEA), Laboratoire Léon Brillouin (LLB) at the Centre d'Etudes de Saclay (20 August 1992 to 20 February 1993).
5. "Directeur de Recherches" Associé at the CNRS. Contract from February 20, 1993 to February 20, 1994. Research activity at LLB, Centre d'Etudes de Saclay (CEA-CNRS).
6. CEA Engineer (E6), "Physicien Chercheur" at Laboratoire Léon Brillouin, Centre d'Etudes de Saclay, from July 1, 1994 up to 28 February 2006. From January 2001 to december 2002 I was also working in the "Service de Physique Statistique, Magnétisme et Supraconductivité" of CEA/Grenoble.
7. Physicist at the Institut Laue-Langevin, Diffraction Group Leader, from March 1, 2006, Grenoble.

## MEMBERSHIP OF SCIENTIFIC INSTITUTIONS AND COMMITTEES

- Coordinator for the Structural Science and Solid State Chemistry group of the Scientific Case of the European Spallation Source project (1995-1996)
- Member of the College 5B, "Magnetism" committee, at the ILL from April 1997 to April 2000.
- Chairman of the College 5B, "Magnetism" committee, at the ILL from April 2000 to October 2001.
- Member of the Neutron Scattering Commission of the International Union of Crystallography (from August 1999).
- Member of the Instrumentation Task Group of the European Spallation Source project.
- Member of the "Comité de Programme" of the French CRG (Collaborative Research Group) beam lines at the ESRF (European Synchrotron Radiation Facility). From October 1999 to December 2003.
- Member of the Scientific Committee of the SINQ neutron facility at PSI from June 2004.
- Member of the AFP-I of the ISIS neutron facility at RAL from June 2005.

## SCIENTIFIC BACKGROUND AND RESEARCH ACTIVITIES

### *Experimental techniques and topics of research before moving to France (1978-1987)*

- Emission Mössbauer Spectroscopy in  $^{57}\text{Co}$ , Electron capture, after-effects, point defects. Absorption Mössbauer Spectroscopy in Spinels, Perovskites and Hexaferrites. Charge states, cationic distribution, cation coordination, anionic vacancies.
- Structure determination by X-ray, Electron and Neutron diffraction. Direct methods, Patterson, Rietveld Method, nuclear and magnetic structures.

- Magnetic properties of oxides. Anisotropy, ferrimagnetism, spin glasses, weak ferromagnetism, small particles.
- High Resolution Electron Microscopy. Anionic Vacancy Ordering in non-stoichiometric perovskites (oxides). Lattice image simulation in HREM, order-disorder, superstructures.
- Energy, potential, electric field and electric field gradient in ionic crystals. Lattice sums, Fourier series, dipolar contribution to the EFG, Bertaut method.

### ***Current scientific interests***

1. - Data analysis and software development in Crystallography and Diffraction Physics.
2. - Theoretical analysis of magnetic Structures. Frustration and low dimensional magnetism.
3. - Physics of Transition Metal-Rare Earth and Superconducting oxides and intermetallics.
  - Metal-Insulator Transitions and Magnetic Ordering in nickel and copper oxides.
  - Magnetic structures of Rare Earth Intermetallics.
  - Structural and magnetic aspects of oxides presenting colossal magnetoresistance and charge, spin and orbital ordering phenomena.

### **Selected representative publications from 1998**

1. "Neutron Diffraction Study of the Magnetic and Orbital Ordering in  $^{154}\text{SmNiO}_3$  and  $^{153}\text{EuNiO}_3$ ". **Physical Review B** **57**, 456 (1998).
2. "Neutron Diffraction Study of the Jahn-Teller Transition in Stoichiometric  $\text{LaMnO}_3$ ". **Physical Review B** **57**, *Rapid Communications*, R3189 (1998)
3. "Liquid-like Spatial Distribution of Magnetic Droplets Revealed by Neutron Scattering in  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ ". **Physical Review Letters** **81**, 1957 (1998).
4. "Electronic Crystallization in a Lithium Battery Material: Columnar Ordering of Electrons and Holes in the Spinel  $\text{LiMn}_2\text{O}_4$ ". **Physical Review Letters** **81**, 4660 (1998).
5. "Magnetic Ordering of  $\text{ErFe}_4\text{Ge}_2$  Studied By Neutron Diffraction and Magnetic Measurements". **Journal of Magnetism and Magnetic Materials** **191**, 261 (1999).
6. "Cubic  $\leftrightarrow$  Orthorhombic Transition in the Stoichiometric Spinel  $\text{LiMn}_2\text{O}_4$ ". **Solid State and Electrochemical Letters** **2**, 6 (1999).
7. "Magnetic Coupling Induced by Hole Doping in Perovskites  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ : A Neutron Scattering Study". **Physical Review B** **60**, 12299 (1999).
8. "Infrared spectroscopy investigation of the charge ordering transition in  $\text{LiMn}_2\text{O}_4$ ". **Solid State Communications** **111**, 453 (1999)
9. "X-Ray study of the spinel  $\text{LiMn}_2\text{O}_4$  at low temperatures". **Chemistry of Materials** **11**, 3629 (1999).
10. "A powder neutron diffraction investigation of the two rhombohedral NASICON analogs:  $\gamma\text{-Na}_3\text{Fe}_2(\text{PO}_4)_3$  and  $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$ ". **Chemistry of Materials** **12**, 525 (2000)
11. The Double Phase Transition on  $\text{ErFe}_4\text{Ge}_2$ . An XRPD Study". **Journal of Magnetism and Magnetic Materials** **210**, 121 (2000).
12. "Evidence of Anisotropic Magnetic Polarons in  $\text{La}_{0.94}\text{Sr}_{0.06}\text{MnO}_3$  by neutron scattering and comparison with Ca-doped Manganites". **Physical Review B** **61**, 9513 (2000).
13. "Structure and Thermal Expansion of the Low Temperature Phase of  $\text{SF}_6$ ". **Low Temperature Physics** **26**, 296 (2000).
14. "Dependence of the Physical Properties of  $\text{Nd}_{0.5}\text{Ca}_{0.5}\text{MnO}_{3+\delta}$  on the Oxidation State of Mn". **Physical Review B** **62**, 3002 (2000).
15. "Simultaneous structural and magnetic transitions in  $\text{YFe}_4\text{Ge}_2$  studied by neutron diffraction and magnetic measurements". **Journal of Magnetism and Magnetic Materials** **236**, 14 (2001).
16. "Crystal and magnetic structure of orthorhombic  $\text{HoMnO}_3$ ". **Physical Review B** **63**, 094411 (2001).
17. "Stability of the Jahn-Teller effect and magnetic study of  $\text{LaMnO}_3$  under pressure". **Physical Review B** **64**, 064426 (2001).
18. "Approach to the metal-insulator transition in  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$  ( $0 \leq x \leq 0.2$ ): Magnetic inhomogeneity and spin-wave anomaly". **Physical Review B** **64**, 104421 (2001).
19. "Crystal and magnetic structures of the oxyphosphates  $\text{MFePO}_5$  ( $\text{M} = \text{Fe}, \text{Co}, \text{Ni}, \text{Cu}$ ). Analysis of the magnetic ground state in terms of superexchange interactions". **The European Physical Journal B** **22**, 429 (2001).

20. "Neutron diffraction study of the magnetic ordering in the series  $R_2\text{BaNiO}_5$  (R=Rare Earth) ". **The European Physical Journal B** **24**, 59 (2001).
21. "Magnetic Structural Studies of the Two Polymorphs of  $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$ : Analysis of the Magnetic Ground State from Super-Super Exchange Interactions". **Chemistry of Materials** **13**, 4527 (2001).
22. "Magnetic structure determination from powder diffraction. Symmetry analysis and simulated annealing". **Materials Science Forum** **378-381**, 268 (2001).
23. "A neutron diffraction study of the antiferromagnetic diphosphate  $\text{LiFeP}_2\text{O}_7$ ". **Solid State Sciences** **4**, 973 (2002).
24. "A new interpretation of the CO state in half-doped manganites: new results from neutron diffraction and synchrotron radiation experiments". **Physica B** **320**, 1 (2002).
25. "Zener Polaron Ordering in Half-Doped Manganites". **Physical Review Letters** **89**, 097205 (2002).
26. "Re-entrant magneto-elastic transition in  $\text{HoFe}_4\text{Ge}_2$ : an XRPD study". **Journal of Magnetism and Magnetic Materials** **250**, 225 (2002)
27. "Magnetic Structures of the Triphylite  $\text{LiFePO}_4$  and of its Delithiated Form  $\text{FePO}_4$ ". **Chemistry of Materials** **15**(21), 4082 (2003).
28. "FullProf as a new tool for flipping ratio analysis". **Physica B: Condensed Matter** **335**, 219 (2003).
29. "Magnetic Properties of Paramelaconite ( $\text{Cu}_4\text{O}_3$ ). A pyrochlore lattice with  $S=1/2$ ". **Physical Review B** **69**, 104408 (2004).
30. "Direct Determination of the Magnetic Ground State in the Square Lattice  $S=1/2$  Antiferromagnet  $\text{Li}_2\text{VOSiO}_4$ ". **Physical Review Letters** **93**, 027202 (2004).
31. "Direct localization of atoms in mixed-occupancy powders by resonant contrast diffraction" **Angewandte Chemie-International Edition** **44**, 1725 (2005)
32. "Ordered spin ice state and magnetic fluctuations in  $\text{Tb}_2\text{Sn}_2\text{O}_7$ ". **Physical Review Letters** **94**, 246402 (2005).
33. "Paramagnetic fluctuations in  $\text{Pr}_{0.65}\text{Ca}_{0.35}\text{MnO}_3$  around the charge-ordering temperature". **Journal of Physics: Condensed Matter** **18**(5), 1509 (2006).
34. "Synchrotron and neutron diffraction study of 4-methylpyridine-N-oxide at low temperature". **Acta Crystallographica B** **62**, 627 (2006).

#### The 10 most cited papers (27 July 2006)

(The figures in parenthesis correspond to the number of *correct* and *bad* citations. For instance in the second paper, there are 99 citations putting the page of the article as "3189", instead of "R3189")

- "Recent Advances in Magnetic Structure Determination by Neutron Powder Diffraction"  
 Juan Rodríguez-Carvajal  
*Physica B* **192**, 55-69 (1993) **1511 (1471+40) citations**
- "Neutron Diffraction Study of the Jahn-Teller Transition in Stoichiometric  $\text{LaMnO}_3$ "  
 J.Rodríguez-Carvajal, M. Hennion, F.Moussa, A.H. Moudden, L. Pinsard and A. Revcolevschi  
*Physical Review B* **57**, *Rapid Communications*, R3189-R3192 (1998) **217 (118+99) citations**
- "Neutron Diffraction Study on Structural and Magnetic Properties of  $\text{La}_2\text{NiO}_4$ "  
 J. Rodríguez-Carvajal, M.T. Fernández-Díaz and J.L. Martínez.  
*Journal of Physics: Condensed Matter* **3**, 3215-3234 (1991) **207 (199+8) citations**
- "Neutron Diffraction Study of  $\text{RNiO}_3$  (R=La, Pr, Nd, Sm). Electronically Induced Structural Changes Across the Metal-Insulator Transition"  
 J.L. García-Muñoz, J. Rodríguez-Carvajal, P. Lacorre and J.B. Torrance.  
*Physical Review B* **46**(8), 4414-4425 (1992) **183 citations**
- "Spin waves in the antiferromagnet perovskite  $\text{LaMnO}_3$ : a neutron scattering study"  
 F.Moussa, M. Hennion, J.Rodríguez-Carvajal, L. Pinsard and A. Revcolevschi  
*Physical Review B* **54** (21), 15149-15155 (1996) **163 citations**
- "Liquid like Spatial Distribution of Magnetic Droplets Revealed by Neutron Scattering in  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ ."  
 M. Hennion, F.Moussa, G. Biotteau, J.Rodríguez-Carvajal, L. Pinsard and A. Revcolevschi  
*Physical Review Letters* **81**, 1957-1960 (1998). **151 citations**
- "Magnetic Frustration and Lattice Dimensionality in  $\text{SrCr}_8\text{Ga}_4\text{O}_{19}$ "

X. Obradors, A. Labarta, A. Isalgué, J. Tejada, J. Rodríguez and M. Pernet.  
*Solid State Communications* **65**(3), 189-192 (1988) **115 citations**

“Electronic Crystallization in a Lithium Battery Material: Columnar Ordering of Electrons and Holes in the Spinel  $\text{LiMn}_2\text{O}_4$ .”

J. Rodríguez-Carvajal, G. Rousse, C. Masquelier and M. Hervieu.  
*Physical Review Letters* **81**, 4660-4663 (1998). **100 (97+3) citations**

“WinPLOT: A Windows tool for powder diffraction pattern analysis.”

T. Roisnel and J. Rodríguez-Carvajal.  
*Materials Science Forum* **378-3**, 118-123 (2001). **98 citations**

"Anomalous Structural Behaviour of Stoichiometric  $\text{La}_2\text{NiO}_4$ "

J. Rodríguez-Carvajal, J. L. Martínez, J. Pannetier and R. Saez-Puche.  
*Physical Review B* **38** (10), *Rapid Communications*, 7148-7151 (1988) **82 (80+2) citations**

**FullProf Citations:** **> 3690 citations**

The use of FullProf is cited in different ways. Some people (mostly those working with magnetic structures) cite directly the paper *Physica B* **192**, 55-69 (1993) (with **1511 citations**), other people just cite the name of the program, the version, the manual, etc (around **990 citations**) and other makes reference to the communication: "FULLPROF: A Program for Rietveld Refinement and Pattern Matching Analysis", by J. Rodríguez-Carvajal, at the *Satellite Meeting on Powder Diffraction of the XV IUCr Congress*, 127 (1990) (around **1190 citations**)