**Proposal for Stephenson Distinguished Visitor Programme**

**Guest scientist**

**Dr. Juan Rodríguez-Carvajal**

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Dr. Juan Rodríguez-Carvajal has been working in the fields of condensed matter physics and crystallography for more than 35 years. His research topics include, among others, powder and single crystal X-ray and neutron diffraction, crystallography and magnetism, as well as the development of software to perform the analysis of data obtained in this type of experiments. He is the author of the [FullProf](https://www.ill.eu/sites/fullprof/php/programs.html) program, one of the most world widely used programs for diffraction data analysis. He has developed his career mainly at Laboratorie Léon Brillouin (LLB, Saclay, France) and at the Institut Laue-Langevin (ILL, Grenoble, France). During his career, he has been invited to more than 90 international events, including workshops and conferences.

His 5 most cited papers according to the Web of Science (April, 11th 2017):

* “Recent Advances in Magnetic Structure Determination by Neutron Powder Diffraction”

Juan Rodríguez-Carvajal

*Physica B* 192, 55-69 (1993)

Citations: 6410

* “WinPLOTR: a Windows tool for powder diffraction patterns analysis”

T. Roisnel and J. Rodríguez-Carvajal.

*Materials Science Forum* 378-381, 118-123 (2001)

Citations: 653

* "Neutron Diffraction Study of the Jahn-Teller Transition in Stoichiometric LaMnO3"

J.Rodríguez-Carvajal, M. Hennion, F.Moussa, A.H. Moudden, L. Pinsard and A. Revcolevschi

*Physical Review B* 57, Rapid Communications, R3189-R3192 (1998)

Citations: 438

* "Neutron Diffraction Study on Structural and Magnetic Properties of La2NiO4"

J. Rodríguez-Carvajal, M.T. Fernández and J.L. Martínez.

*Journal of Physics: Condensed Matter* 3, 3215-3234 (1991)

Citations: 350

* "Neutron Diffraction Study of RNiO3 (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)

Citations: 349

**Host scientist(s)**

**Dr. Sonia Francoual**, Beamline scientist in charge, beamline P09, PETRA III, FS-PE

**Dr. Pablo J. Bereciartua**, Post-doctoral research associate, beamline P09, PETRA III, FS-PE

**Details of the proposed visit at DESY Photon Science in Hamburg**

The proposed visit would last 2 weeks in 2018. The funding request would cover the travel and the staying expenses for this period.

**Scientific programme during the visit**

Resonant X-ray magnetic scattering (RXMS) is a powerful technique to probe magnetic structures either in complement to neutron diffraction when more than one magnetic ions order in a material or as an alternative when the sample growth process does not allow it to grow large enough samples to allow for neutron studies or when the ordering ions present too large an absorbing cross-section. Despite the many years since the establishment of the RXMS technique and the construction of dedicated beamlines and instruments, no tools have been yet made available to the user community to analyze RXMS data restraining its use to few knowledgeable groups and limiting its worldwide reach. We have initiated a new project at the Resonant Scattering and diffraction P09 beamline of PETRA III aiming at providing the user community with software allowing for magnetic structure determination from RXMS data. This software will be developed by Dr. Bereciartua based on the Crystallographic Fortran Modules Library ([CrysFML](https://forge.epn-campus.eu/projects/crysfml)), whose main author is Dr. Rodríguez-Carvajal, who agreed to collaborate in the development of the described software and on python and mathematica scripts previously written by P09 staff for that purpose (Dr. Sonia Francoual and Dr. Jose Linares Mardegan). The proposed stay of Dr. Rodríguez-Carvajal at DESY will allow to check on advances (project started August 1st), give him the opportunity to get to know the P09 instrument and discuss possible future case studies.

**Existing or possible future collaboration**

As explained above, there exists an ongoing collaboration between the P09 beamline team and Dr. Rodríguez-Carvajal. The aim of the proposed visit at DESY would be to enhance this collaboration. The outcomes of this collaboration would be beneficial not only to the P09 beamline, but also to the PETRA III users, since the resulting software will facilitate their research at DESY.