

ROBERT J. PAPOULAR (France)

**CEA : Commissariat à L' Energie Atomique
IRAMIS / Laboratoire Léon Brillouin**

Date of Birth: 1 September 1953

CEA-CEN Saclay Place of Birth: Paris, France

91191 Gif-sur-Yvette, France Nationality : French

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Family status : Married, 2 children

CURRENT RESEARCH INTERESTS

Molecular and Pharmaceutical Compounds

X-Ray / Neutron diffraction

Single-Crystal / Powder diffraction

Crystallographic Imaging & Data Analysis

IR Spectroscopy , UV Spectroscopy

Graphene & Graphite

Molecular Modeling

EDUCATION

Habilitation, Chemical Physics, Faculty of Pharmacy, University Paris 5, 2006 :
Thesis : Radiocrystallography of molecular compounds and of compounds of
pharmaceutical interest, Advisor: Prof. René Céolin

Ph.D., Solid State Physics, Faculty of Sciences, University Paris 11, 1992
Thesis : Neutron Spin Echo spectroscopy. Its application to the study of the
dynamics of polymers in solution, Advisor: Prof. Marianne Lambert

DEA in Solid State Physics, University Paris 11 [Prof. J. Friedel], 1977

Engineering Diploma [major: Physics] from **Ecole Centrale Paris**, 1976
[**Ecole Centrale des Arts et Manufactures**,
(One of the top 5 High Tech Schools in France)]

PROFESSIONAL EXPERIENCE

Léon Brillouin Laboratory, CEA-Saclay, Senior Physicist [E5 band, 2000],[E6 band, 2008] (Max is E7, for Heads).

Brookhaven National Laboratory, New-York, USA, Invited Visiting Scientist, 1993-1995.

Invited by the Physics Department [Principal Investigator : Dr. David E. Cox].

Léon Brillouin Laboratory, CEA-Saclay, Tenured Physicist since 1982.

Project leader, beamline scientist, responsible for building, running, managing a Neutron Spin Echo spectrometer (1982-1992).

Léon Brillouin Laboratory, CEA-Saclay, Experimentalist Scholarship (CEA/CFR), 1977-1979,1980-1982 [1979-1980 : Military Duty at DRET/ DRI Paris, French Air Force]

CEA : Commissariat à l' Energie Atomique, is the French equivalent of the US DOE (Department of Energy).

SCIENTIFIC PANEL MEMBERSHIP

Rutherford-Appleton Laboratory (RAL) / ISIS / UK. Diffraction panel: 11/1996 - 6/1999

Institut Laue-Langevin (ILL) / Grenoble, France. Instrumentation Committee: 1987 – 1989

Helmholtz Zentrum Berlin (HZB) / Berlin, Germany. Member of the Science Selection Panel [Photons & Neutrons - Panel C6 : Hard Condensed Matter]: 2012 – 2017 (?)

SCIENCE MEMBERSHIP

Member of the APS since 1987 [American Physical Society]

Member of the ACA since 1994 [American Crystallographic Association]

Member of the NSSA since 1993 [Neutron Scattering Society of America]

Member of the SIMP since 2006 [Societa Italiana di Mineralogia e Petrologia]

Member of the ICDD since 2010 [International Centre for Diffraction Data]
Chairman of one of the ICDD technical subcommittees : " X-ray Diffraction Methods "
+ Director at-Large / Board of Directors since March 2014

Faculty Member of the ACA Summer Course since July 2011

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PUBLICATIONS

Over 65 refereed publications, including 11 letters [PRL: 3; CPL: 3, EPL: 4, AAL: 1].

The list of Letters is attached hereafter.

So is a list of recent publications in Journals with High Impact Factors [> 4.5].

INVITED INTERNATIONAL CONFERENCES

Over 19, including: IUCr Congresses (3); ACA(1, USA); BCA (2, UK); Gordon Conf. (2,USA), Sagamore Conf. (2).

INVITED LECTURER AT INTERNATIONAL SCHOOLS

"Current Problems in Condensed Matter Research", Bialowieza, Poland, 1993.

"Recent Developments in Neutron Scattering", Les Houches, France, 2000.

"Polarized Neutrons in Materials and Life Sciences", Anglet, France, 2005.

"American Crystallography Association Summer Course", since 2011.

REVIEWER

Regular referee for : PRL, PRB, CPL, ActaCryst A & B since 1995.

Occasional referee for : Chemistry of Materials, Philosophical Magazine, Physica Scripta, Carbon, Journal of Powder Diffraction, ...

TECHNICAL ACCOMPLISHMENTS

Crystallographic Imaging from X-ray / Neutron Powder / Single-Crystal data.
Accurate Charge & Spin Densities [1990-2008].

The ILL [Grenoble , France] Maximum Entropy software with which the neutron diffraction polarized data are routinely analyzed since 1992 is largely based on my initial code and results from a collaboration over many years between Dr. J. Schweizer (ILL) and myself.

This original work captured Dr. D.E. Cox's and Prof. P. Coppens' interests. The former invited me to BNL / NSLS to transpose it to X-ray powder data, while the latter later invited me for shorter terms to SUNY/ Buffalo to apply it to Accurate Charge Densities

borne from single-crystal data. Most of my invited international conferences and letters result from this activity.

Construction and commissioning of the MESS [Machine à Echos de Spins de Saclay] Neutron Spin Echo spectrometer at the Orphée Reactor / CEA-Saclay [1982-1992].

At the time, this spectrometer was in fact the second of its kind in the world, after the very first IN11 ILL NSE instrument. It was built in the framework of a collaboration between Prof. F. Mezei [Hungarian Academy of Science] and LLB / CEA-Saclay. Initially intended to measure diffusive motion, this instrument was diverted from its initial goal to measure Tc with polarized neutrons for the first time in a high-Tc superconductor [Papoular & Collin, PRB, 1988], a procedure later used by American colleagues.

Two long term US visitors ca 1987: S.M. Shapiro [BNL/NY] and R.N. Silver [LANL / NM] have come to learn about the NSE technique while this instrument was being completed.

Development of a hydrostatic high-pressure cell up to 25 Kbar for neutron diffraction experiments [1977-1985].

[This project was initiated by a collaboration with Prof. Daniel L. Decker (Brigham Young University, Utah) during his sabbatical leave in France ca 1977-1978.]

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Selected Publications (Letters)

1. R.J. Papoular, B. Gillon, "Maximum Entropy reconstruction of spin density maps in crystals from polarized neutron diffraction data."
Europhys. Lett. 13, 429 (1990).
2. M. de Boissieu, R.J. Papoular, C. Janot, "Maximum-Entropy as applied in Quasi-Crystallography."
Europhys. Lett. 16, 343 (1991).
3. R. Papoular, J. Breton, G. Gensterblum, I. Nenner, R.J.Papoular, J.-J. Pireaux, "The vis/UV spectrum of coals and the interstellar extinction curve."
Astron. Astrophys. L5-L8, 270 (1993).
4. R.J. Papoular, A. Delapalme, "Model-free polarized neutron diffraction study of an acentric crystal."
Phys. Rev. Lett. 72, 1486 (1994).
5. R.J. Papoular, D.E. Cox, "Model-free search for extra-framework cations in zeolites using powder diffraction."
Europhys. Lett. 32, 337 (1995).

6. P. Schiebel, R.J. Papoular, W. Paulus, H. Zimmermann, A. Detken, U. Haebleren, W. Prandl, "Isotope induced proton ordering in partially deuterated aspirin.", *Phys. Rev. Lett.* 83, 975 (1999).
7. V.H. Plakhty, A.G. Gukasov, R.J. Papoular, O.P. Smirnov, "Spin density on ligands O²⁻ and covalency of Fe⁺³ ions in octahedral sites of the Ca₃Fe₂Ge₃O₁₂ garnet: a polarized neutron diffraction study." *Europhys. Lett.* 48, 233 (1999).
8. A. Gukasov, M. Braden, R.J. Papoular, S. Nakatsuji, Y. Maeno, "Anomalous Spin Density Distribution on Oxygen and Ruthenium in Ca_{1.5}Sr_{0.5}RuO₄." *Phys. Rev. Lett.* 89, 087202 (2002).
9. R. Ceolin, D.O. Lopez, M. Barrio, J. Ll. Tamarit, P. Espeau, B. Nicolai, H. Allouchi, R.J. Papoular, "Solid state studies on C₆₀ solvates formed with n-alkanes: orthorhombic C₆₀.2/3 n-nonane." *Chem. Phys. Lett.* 399, 401 (2004).
10. R. Le Parc, C. Levelut, J. Haines, V. Davydov, A.V. Rakhmanina, R.J. Papoular, E.E. Belova, L.A. Chernozatonskii, H. Allouchi, V. Agafonov, "In situ X-ray powder diffraction study of one-dimensional polymeric C₆₀ phase transformation under high-pressure." *Chem. Phys. Lett.* 438, 63 (2007).
11. R.J. Papoular, B.H. Toby, V.A. Davydov, A.V. Rakhmanina, A. Dzyabchenko, H. Allouchi, V. Agafonov, "Single-crystal and synchrotron X-ray powder diffraction study of the one dimensional orthorhombic polymer phase of C₆₀." *Chem. Phys. Lett.* In press (2008).

Selected Recent Publications since 2009 [with High Impact Factor > 4.5] :

- [1] R.J. Papoular & R. Papoular, "A polycrystalline graphite model for the 2175 Å interstellar extinction band." *MNRAS*, 394, 2175 (2009) [IF = 5.521]
- [2] R.J. Papoular, S. Yuan, R. Roldán, M.I. Katsnelson and R. Papoular, "Effects of structural and chemical disorders on the vis/UV spectra of carbonaceous interstellar grains." *MNRAS*, 432, 2962 (2013) [IF = 5.521]
- [3] L. Fajari, R.J. Papoular, M. Reig, E. Brillas, J.L. Jorda, L. O. Vallcorba, J. Rius, D. Velasco and L. Juliá, "Charge Transfer States in Stable Neutral and Oxidized Radical Adducts from Carbazole Derivatives," *J. Org. Chem.*, 79, 1771 (2014) [IF = 4.564]
- [4] R.J. Papoular & R. Papoular, "Some optical properties of graphite from IR to millimetric wavelengths." *MNRAS*, accepted (2014) [IF = 5.521]