

## RÉSUMÉ

LIC. JUAN E. PERALTA

PHYSICS DEPARTMENT, FCEYN UBA  
 CIUDAD UNIVERSITARIA PAB. 1  
 BUENOS AIRES 1428, ARGENTINA  
 EMAIL: [juanp@df.uba.ar](mailto:juanp@df.uba.ar)

OCTOBER 2001

### PERSONAL DATA

Date of Birth	April 29, 1971
Nationality	Argentine
Marital Status	Married to Verónica Barone, 1 child coming
Private address	Coronel Niceto Vega 4601 Buenos Aires (1414) Argentina
Phone	+54(11) 4775-2841
e-mail	<a href="mailto:juanp@df.uba.ar">juanp@df.uba.ar</a>

### EDUCATION

1983-1989	High School: National College of Buenos Aires, UBA.
1990 - 1997	Licenciado en Física (M. Sc. in Physics), UBA.
Oct 1997 - present	PhD. studies in the Physics Department, University of Buenos Aires (UBA), Advisor: Prof. Dr. Rubén. H. Contreras, <a href="mailto:contrera@df.uba.ar">contrera@df.uba.ar</a> .
Graduate Courses	<ul style="list-style-type: none"> <li>• Methods in Quantum Chemistry (1997)</li> <li>• Introductions to Solid State Physics II (1998)</li> <li>• Laboratory of Electronics (2001)</li> <li>• Non Linear Dinamics (2001)</li> <li>• Many Bodies Quantum Theory (2001)</li> </ul>
Other Courses	<ul style="list-style-type: none"> <li>• Workshop: Introduction to Gaussian: Theory and practice, Buenos Aires 1997.</li> <li>• The Ab Initio Calculation of Molecular Properties (Stephan Sauer), Corrientes 2001</li> <li>• NMR of Solids: Principles &amp; Applications (Robin K. Harris), Corrientes 2001</li> <li>• Density Functionals (Patricio Fuentealba), Corrientes 2001</li> </ul>

---

**FELLOWSHIPS**


---

- Oct 1997 - Set 1999 "Initiation to Research" fellowship from the National Council of Scientific and Technologic Researches (CONICET).
- Oct 1999 - Set 2001 Fellowship from CONICET to continue PhD. studies.
- Oct 2001 - Set 2002 Fellowship from CONICET to finish PhD. studies.

---

**TEACHING EXPERIENCE**


---

- Mar 1999 - present Professor of *Environmental Physics* in the "Universidad de Ciencias Empresariales y Sociales" (UCES), Argentina.
- Ago 1998 - present Teaching assistance in the Physics Department, UBA
- Jun 1996 - Dec 1997 Professor of Physics in the high school *Escuela del Caminante*.
- Mar 1996 - Mar 1997 Teaching assistance in the Physics Department, UBA
- Jun 1992 - Jun 1993 Teaching assistance in the preparatory course, UBA

---

**PUBLICATIONS**


---

- (1) 2001 Mol Phys, in press Daniel G. Zaccari, James P. Snyder, Juan E. Peralta, Oscar E. Taurian, Rubén H. Contreras and Verónica Barone, "*Natural J Coupling (NJC) Analysis of the Electron Lone Pair Effect on NMR Couplings 2. The Anomeric Effects on  $^1J(C,H)$  Couplings and its Dependence on Solvent*"
- (2) 2001 J Am Chem Soc 123, 9162-9163 Juan E. Peralta, Verónica Barone, Rubén H. Contreras, Daniel G. Zaccari and James P. Snyder, "*Through-Bond and Through-Space  $J_{FF}$  Spin-Spin Coupling in Peri-difluoronaphthalenes: Accurate DFT Evaluation of the Four Contributions*"
- (3) 2001 J Phys Chem A 105, 5298-5303 A. L. Esteban, M. P. Galache, F. Mora, E. Díez, J. Casanueva, J. San Fabián, V. Barone, J. E. Peralta and R. H. Contreras, "*Vicinal NMR Proton-Proton Coupling Constants. An NBO Analysis*"
- (4) 2001 Magn Reson Chem 39, 600-606 V. Barone, J. E. Peralta, R. H. Contreras, A. V. Sosnin and L. B. Krivdin, "*Natural J Coupling (NJC) Analysis of the Electron Lone Pair Effect on NMR Couplings. 1: The Lone Pair Orientation Effect of an  $\alpha$ -Nitrogen Atom on  $^1J(C,C)$  Couplings*"
- (5) 2001 J Comput Chem 22, 1615-1621 V. Barone, J. E. Peralta and R. H. Contreras, "*NMR  $^3J(C1,H3)$  Couplings in 1-X-bicyclo[1.1.1]pentanes. FPT-DFT and NBO Studies of Hyperconjugative Interactions and Heavy Atom Substituent Effects*"

- (6) 2001 Mol Phys 99, 655-661 J. E. Peralta, V. Barone, M. C. Ruiz de Azúa and R. H. Contreras, "FPT-DFT Calculation of the Spin-Dipolar Contribution to NMR Spin-Spin Coupling Constants"
- (7) 2000 Prog NMR Spectroscopy 34(4), 321-425 R. H. Contreras and J. E. Peralta, "Angular Dependence of Spin-Spin Coupling Constants"
- (8) 2000 J Mol Struct 556, 263-273 R. H. Contreras, O. E. Taurian, F. S. Ortiz and J. E. Peralta, "The Polar Bond-Polarizable Bond Interaction in 1-X,2-Methoxy Naphthalenes. An Experimental and Theoretical Study"
- (9) 2000 Theoret Chem Acc 105, 165-168 Juan E. Peralta, Martín C. Ruiz de Azúa and Rubén H. Contreras, "On the Convergence of FPT-DFT Calculations of the Fermi Contribution to NMR Coupling Constants (Letter)"
- (10) 2000 Magn Reson Chem 38, 395-402 E. W. Della, I. J. Lochert, J. E. Peralta, and R. H. Contreras, "Theoretical and Experimental Study of  $^{13}\text{C}$  SCSs in 1-X-Biciclo[1.1.1]Pentanes"
- (11) 2000 Chem Commun 20, 2025-2026 J. E. Peralta, R. H. Contreras and J. P. Snyder, "Natural Bond Orbital Dissection of Fluorine-Fluorine Through-Space NMR Coupling ( $J_{F,F}$ ) in Polycyclic Organic Molecules"
- (12) 1999 J Mol Struct Theochem 491, 23-31 J. E. Peralta, M. C. Ruiz de Azúa and R. H. Contreras, "Natural Bond Orbitals analysis of C—H...O interactions in NCH/H<sub>2</sub>O and NCH/OCH<sub>2</sub>, and their effect on nuclear magnetic shielding constants"
- (13) 1999 Magn Reson Chem 37, 167-172 W. Adcock, D. Lünsmann, J. E. Peralta and R. H. Contreras, "DFT-GIAO and NBO studies of the origin of 19-F shielding effects in alkyl fluorides"
- (14) 1999 Magn Reson Chem 37, 227-231 D. G. de Kowalewski, V. J. Kowalewski, J. E. Peralta, G. Eskuche, R. H. Contreras, A. L. Esteban, M. P. Galache and E. Díez, "Intramolecular electric field effect on a 1-J(CH) NMR spin-spin coupling constant. An experimental and theoretical study"
- (15) 1999 Magn Reson Chem 37, 31-35 J. E. Peralta, R. H. Contreras, O. E. Taurián, F. S. Ortiz, D. G. de Kowalewski and V. J. Kowalewski, "Methyl  $\beta$  substituent effect on  $^{17}\text{O}$  chemical shifts in two-coordinated oxygen atoms: DFT GIAO and NBO, and experimental studies"
- (16) 1998 Int J Quantum Chem 70, 105-112 J. E. Peralta, M. C. Ruiz de Azúa and R. H. Contreras, "Electrostatic effect of the polar bond – polarizable bond interaction on  $^{13}\text{C}$  chemical shifts"

---

**CHAPTERS IN BOOKS**


---

"Advances in Theoretical and Physical Aspects of Spin-Spin Coupling Constants", R. H. Contreras, J. E. Peralta, C. G. Giribet, M. C. Ruiz de Azúa and J. C. Facelli, Annual Reports on NMR Spectroscopy Vol. 41(2000), pags. 55-184.

---

**POSTERS**


---

*International Meetings*

- |      |   |  |
|------|---|--|
| 2000 | XVII Simposio Iberoamericano de Catálisis, Porto, Portugal.                         | M. M. Branda, J. E. Peralta, N. J. Castellani y R. H. Contreras, "Adsorción de Metanol sobre un catalizador modelo de Oxido de Magnesio"   |
| 1999 | 5 <sup>th</sup> World Congress of Theoretically Oriented Chemists, London, UK.      | R. H. Contreras, J. E. Peralta, A. Esteban, and E. Díez, "Analysis of Electron Delocalization Effects on <sup>2</sup> J(CH) and <sup>2</sup> J(HH) NMR Coupling Constants: an NBO Approach"  |
| 1998 | 29 <sup>th</sup> AMPERE - 13 <sup>th</sup> ISMAR International Conference, Berlin.  | Kowalewski, D. G. de; Esteban, A. L.; Galache, M. P.; Díez, E.; Kowalewski, V. J.; Peralta, J. E.; Eskuche, G. and Contreras, R. H., "Intramolecular electric field effect on a 1J(CH) NMR spin-spin coupling constant. An experimental and theoretical study" |
| 1998 | Sanibel Symposium, Ponce de Leon, Florida, USA.                                     | Juan E. Peralta; Martín C. Ruiz de Azúa and Rubén H. Contreras, "Natural Bond Orbitals analysis of C—H...O interactions in NCH/H <sub>2</sub> O and NCH/OCH <sub>2</sub> , and their effect on nuclear magnetic shielding constants"                           |
| 1997 | 9 <sup>th</sup> International Congress of Quantum Chemistry, Atlanta, Georgia, USA. | Juan E. Peralta; Martín C. Ruiz de Azúa and Rubén H. Contreras, "Electrostatic effect of the polar bond - polarizable bond interaction on <sup>13</sup> C chemical shift"  |

*National Meetings (Argentina)*

- |           |   |  |
|-----------|---|--|
| 1994-2000 | 16 presentations in the Annual Meetings of the Argentinean Physicists Society |  |
| 1999      | XI Argentinean Meeting on Catalysis   | M. M. Branda, J. E. Peralta, N. J. Castellani y R. H. Contreras, "Adsorción de Metanol sobre un catalizador modelo de Oxido de Magnesio" |

---

**SCIENTIFIC VISITS**


---

- |                      |   |
|----------------------|---|
| Mar 31 - May 4, 2001 | Department of Chemistry, Emory University, Atlanta GA, USA (James. P. Snyder, <a href="mailto:snyder@heisenbug.chem.emory.edu">snyder@heisenbug.chem.emory.edu</a> ). |
| Jul 9 - Jul 31, 2000 | Department of Chemistry, Emory University, Atlanta GA, USA (James. P. Snyder, <a href="mailto:snyder@heisenbug.chem.emory.edu">snyder@heisenbug.chem.emory.edu</a> ). |

Mar 29 - May 4, 1999 Department of Applied Physical Chemistry, Universidad Autónoma de Madrid, Spain (Ernesto Díez Villanueva, [ernesto.diez@uam.es](mailto:ernesto.diez@uam.es)).

Mar 31 - Apr 30, 1998 Center for High Performance Computing, University of Utah, Salt Lake City, USA (Julio C. Facelli, [facelli@chpc.utah.edu](mailto:facelli@chpc.utah.edu)).

---

#### **INTERESTS AND ACTIVITIES**

---

Photography, Soccer, Ping-Pong.