

# Curriculum Vitae

## Datos Personales

Nombre y Apellido: Daniel Héctor LARIA  
Fecha de nacimiento: 3 de setiembre de 1955  
Nacionalidad: Argentina

## Títulos Académicos Universitarios:

Licenciado en Cs. Físicas. FCEN-Universidad de Buenos Aires(1982)  
Doctor of Philosophy in Chemistry. University of California at Berkeley. Berkeley, California, EEUU (1987)

## Posiciones post-doctorales:

Centre Européen de Calcul Atomique et Moléculaire. Orsay- Francia (1991-1992)  
Becario de la Mobility Program de la UE (1992) Dipartimento di Física. Università di Roma. (1992-1993)

## Actividad Profesional

- Investigador A-8. Unidad Actividad Física- Comisión Nacional de Energía Atómica de la Argentina (1980- )
- Profesor Titular Regular. Dedicación simple – Departamento de Química Inorgánica Analítica y Química Física. Facultad de Cs. Exactas y Naturas. Universidad de Buenos Aires (2007- )
- Profesor Visitante. Depto de Física Atómica y Molecular. Universidad Politécnica de Cataluña. Barcelona. España. (Enero-Agosto de 2003)
- Miembro de la carrera del Investigador Científico del CONICET con categoría de Investigador Principal.

## Formación de recursos humanos:

### i) Trabajos finalizados

Ha dirigido cuatro tesis de licenciatura en Cs. Físicas – Dto. de Física – FCEN – UBA

Lic. Silvia Pascale (Junio de 1995)

Lic. Pablo Rusjan (Abril de 1997)

Lic. M. D. Elola. (Mayo 1998)

Lic. A. Tamashiro (Mayo de 2002)

Ha dirigido seis tesis doctorales en Cs. Químicas. DQIAQF, FCEN-UBA

Dr. Mario RE. Diciembre de 1997

Dra. Valeria MOLINERO. Diciembre de 1999

Dr. Pablo RUSJAN. Julio de 2002

Dra. M. Dolores ELOLA. Diciembre de 2002

Dr. Javier RODRÍGUEZ. Diciembre de 2002

Dr. Diego PANTANO. Julio de 2005

## ii) Trabajos en curso

Actualmente dirige dos tesis doctorales de becarios con soporte económico del CONICET (Lic. E. Clavero, Lic. M. Pomata)  
 Director de un Investigadores CONICET (Dr. J. Rodríguez, 2005-)

## Otras actividades:

Miembro asociado del International Centre of Theoretical Physics (Trieste, Italia)  
 Revisor del Journal of Chemical Physics y Journal of Physical Chemistry.  
 Jurado de Tesis de Doctorado (DQIAQF y DF, FCEN) y tesis de Licenciatura (DF-FCEN)

## Titularidad de Subsidios:

Ha recibido 8 subsidios otorgados por la Fundación Antorchas (Argentina) para reinserción en el país, para apoyo a la investigación y para colaboración grupos de Canadá y Brasil (Antorchas/Vitae).

En estos momentos es titular del PIP (CONICET), un proyecto plurianual subvencionado por la ANPCyT (Argentina) y un proyecto UBACyT.

## Presentaciones a congresos:

Más de 6 presentaciones en congresos locales del a AAIFQ y AFA e internacionales incluyendo: Gordon Research Conferences 1998,1999,2001-2003, STATPHYS-17 (1987), Intl. Symposium on othe small particle and inorganic clusters (Lausana, 1998), Intl. Congress of DFT applications (Roma 1999 y Menton 2000)

Conferencista invitado en:

“Quantum Aspects of Diffusion” Eurconference on Technical advances in particle-based Computational Material Science. (Villa Marigola, Lericci- Italia , Julio de 1997).

“Protons in Supercritical Water” Pacifichem 2005. (Honolulu – EE.UU. Diciembre de 2005)

## Publicaciones científicas.

Las publicaciones 14, 15, 25 y 57 corresponden a capítulos en libros. El resto corresponde a publicaciones internacionales **con referato**.

1 - R. Crovetto, M. L. Japas, **D. Laria** y R. Fernández Prini

“Thermodynamics of dissolution of simple gases in water” Accounts of Chemical Research **18**, 207 (1985)

2 - **D. Laria** y D. Chandler

“Comparative study of theory and simulation calculations of excess electrons in simple fluids”. Journal of Chemical Physics. **87**, 4088 (1987)

3 - **D. Laria** y F. Vericat

“Percolative behavior of long permeable objects: a reference interaction site model study” Physical Review B. **40**, 535 (1989).

- 4 - **D. Laria** , H. R. Corti y R. Fernández Prini  
"The cluster theory of electrolyte solutions" Transactions of the Faraday Society. **86** 1051 (1990)
- 5 - **D. Laria** y F. Vericat  
"Clustering and percolation in dipolar hard sphere fluids". Physical Review A. **43**, 1932 (1991)
- 6 - **D. Laria** y R. Fernandez Prini  
"Use of the RISM perturbation method to describe dissolution of non-polar gases in molecular liquids". Journal of Chemical Physics. **94**, 2272 (1991}
- 7 - **D. Laria**, D. Wu y D. Chandler  
"RISM-Polaron theory of hydrated electrons" Journal of Chemical Physics **95**, 4444 (1991)
- 8 - **D. Laria**, G. Ciccotti, M. Ferrario y R. Kapral  
"Molecular dynamics study of adiabatic proton-transfer reactions in solution". Journal of Chemical Physics **97**, 378 (1992).
- 9 - **D. Laria** y R. Fernández-Prini  
"Ion pair solvation in aqueous clusters". Chemical Physics Letters **205**, 260 (1993).
- 10 - **D. Laria**, G. Ciccotti, M. Ferrario y R. Kapral  
"Proton Transfer in Solution". Publicado en Lectures on Thermodynamics and Statistical Mechanics. Proceeding of XXII Winter Meeting in Statistical Physics, Oaxtepec, Mexico. Eds. M. López de Haro and C. Varea. (World Scientific, Singapore, 1994)
- 11 - **D. Laria**, G. Ciccotti, M. Ferrario y R. Kapral  
"Activation free energy for proton transfer in solution". Chemical Physics **180**, 181 (1994).
- 12 - M. Ferrario, **D. Laria**, G. Ciccotti y R. Kapral  
"Quantum Effects on the Solvent Contribution to the Activation Free Energy". Journal of Molecular Liquids **61**, 37 (1994).
- 13 - **D. Laria** y R. Fernandez-Prini  
"Molecular Dynamics study of water clusters containing ion pairs: from contact to dissociation" Journal of Chemical Physics **102**, 7664 (1995).
- 14 - G. Ciccotti, M. Ferrario, **D. Laria** y R. Kapral.  
"Simulation of classical and quantum activated processes in condensed phases" publicado en *Progress in Computational Physics of Matter: Methods, Software and Applications*. Eds. F. Manghi y L. Reatto. World Scientific Co. Singapore (1995).
- 15 - **D. Laria** y R. Fernández-Prini  
"Ions in steam and in aqueous clusters" Proceeding 12th. International Conference on the Properties of Water and Steam. Orlando, Florida (1995). EE.UU.
- 16 - H. R. Corti, **D. Laria** y L. Trevani  
"Ionic association in asymmetric electrolytes" Transactions of the Faraday Society **92**, 93 (1996).
- 17 - M. Re, **D. Laria** y R. Fernández-Prini  
"Solvent structural contributions to the dissolution process of an apolar solute in water" Chemical Physics Letters **250**, 25 (1996).
- 18 - **D. Laria**, R. Kapral, D. Estrin y G. Ciccotti  
"Molecular Dynamics study of solvation effects on acid dissociation in aprotic media" Journal of Chemical Physics **104**, 6560 (1996).

- 19 - M. Margulis, **D. Laria** y R. Fernández-Prini  
"Ionic aggregates in Steam I: Equilibrium configurations" Transactions of the Faraday Society **92**, 2703 (1996).
- 20 - M.Re, **D. Laria** y R. Fernandez-Prini  
"The role of solvent structure in perturbation methods applied to the dissolution process of apolar solutes in water" Berichte der BunsenGessellschaft **100**, 1328 (1996).
- 21 - M. Re y **D. Laria**  
"Solvation effects on a model  $\text{SN}_2$  reaction in aqueous clusters" Journal of Chemical Physics **105**, 4556 (1996)
- 22 - R. Kapral, S. Consta y **D.Laria**  
"Proton Transfer in Clusters" Canadian Journal of Chemistry **75**, 1, (1997).
- 23 - M. Re y **D. Laria**.  
"Dynamics of solvation of supercritical water" Journal of Physical Chemistry, **101**, 10494 (1997).
- 24 - D. Estrin, J. Kohanoff, **D. Laria** y R. Weth  
"Hybrid Quantum and Classical Monte Carlo Simulations of the interaction of Hydrogen Chloride in solid Water Clusters" Chemical Physics Letters, **280**, 280 (1997)
- 25 - **D. Laria**, G. Ciccotti, D. Coker, R. Kapral y M. Ferrario.  
"Non adiabatic methods for diffusion" publicado en Classical and Quantum Dynamics in Condensed Phase Simulations". Editores: B. J. Berne, G. Ciccotti y D. F. Coker. World Scientific, Singapore. (1998).
- 26 - V. Molinero, **D. Laria** y R. Kapral.  
"Mixing and Segregation in Binary Polar-Molecule Clusters" Journal of Chemical Physics **109**, 6844 (1998).
- 27 - J. Rodriguez, **D. Laria**, E. Marceca y D. Estrin.  
"Isomerization, melting, and polarity of model water clusters:  $(\text{H}_2\text{O})_6$  and  $(\text{H}_2\text{O})_8$ " Journal of Chemical Physics. **110**, 9039 (1999)
- 28 - **D. Laria** y M. S. Skaf  
"Solvation Response of Polar Liquid Mixtures: Water-Dimethylsulfoxide" Journal of Chemical Physics. **111**, 300 (1999).
- 29 - D. Elola, D. Estrin y **D. Laria**  
"Hybrid Quantum-Classical Molecular Dynamics Simulation of Proton Transfer Reaction of  $\text{OH}^-$  with  $\text{HBr}$  in Aqueous Clusters" Journal of Physical Chemistry A. **103**, 5105 (1999)
- 30 - V. Molinero, **D. Laria** y R. Kapral  
"Dynamics of solvation-induced structural transitions in mesoscopic polar clusters" Physical Review Letters **84**, 455 (2000)
- 31 - J. Kohanoff, S. Koval, D. Estrin, **D. Laria** y Y. Abashkin.  
"Concertedness and solvent effects in múltiple proton transfer reactions: The formic acid dimer in solution" Journal of Chemical Physics. **112**, 9498 (2000)
- 32 - M. S. Skaf y **D. Laria**  
"Dielectric Relaxation of Supercritical Waters: Computer Simulations" Journal of Chemical Physics. **113**, 3499 (2000)
- 33 - M. D. Elola, E. J. Marceca, **D. Laria** y D. Estrin  
"Computer Simulation Study of  $\text{HNO}_3$  dissociation in aqueous clusters". Chemical Physics Letters. **326**, 509 (2000)

- 34 - **D. Laria**, J. Rodríguez, C. Dellago y D. Chandler  
"Dynamical aspects of isomerization and melting transitions in [H<sub>2</sub>O]<sub>8</sub>" Journal of Physical Chemistry A. **105**, 2646, 2001
- 35- A. Tamashiro, J. Rodriguez y **D. Laría**.  
"Equilibrium and dynamical aspects of solvation of Coumarin-151 in polar nanoclusters"  
Journal of Physical Chemistry A. **106**, 215 (2002)
- 36- J. Rodriguez, G. Moriena y **D. Laria**  
"Dynamical Pathways for isomerization processes in the water nonamer".  
Chemical Physics Letters. **356**, 147 (2002)
- 37 - D. Elola y **D. Laria**  
"Solvation dynamics following electron photodetachment from I<sup>-</sup> in aqueous clusters" Journal of Chemical Physics. **117**, 2238 (2002)
- 38 - **D. Laria** y M. Skaf  
"Path Integral Molecular Dynamics study of electronic states in supercritical water". Journal of Physical Chemistry A. **106**, 8066 (2002)
- 39 - **D. Laria** y R. Kapral  
"Electron solvation in aqueous reverse micelles: equilibrium properties". Journal of Chemical Physics **117**, 7712 (2002)
- 40 - D. A. Pantano y **D. Laria**  
"Solvation dynamics of Coumarin-314 at the water/air interface". Journal of Physical Chemistry B. **107**, 2971 (2003)
- 41 - L. R. Martins, A. Tamashiro, **D. Laria** y M. Skaf.  
"Solvation Dynamics of Coumarin 153 in Dimethylsulfoxide-Water Mixtures: Molecular Dynamics Simulations". Journal of Chemical Physics. **118**, 5955 (2003)
- 42 - J. Rodriguez, M. Skaf y **D. Laria**  
"Equilibrium and dynamical aspects of solvation of excess electrons in supercritical ammonia". Journal of Chemical Physics. **119**, 6044 (2003)
- 43 - **D. Laria**, J. Martí y E. Guàrdia  
"Protons in supercritical water: an empirical valence bond study". Journal of the American Chemical Society. **126**, 2125 (2004)
- 44 - J. Rodriguez y **D. Laria**.  
"Electronic States at the water/air interface". Journal of Physical Chemistry B. **109**, 6473 (2005)
- 45 - D. Pantano, M. Sonoda, M. Skaf y **D. Laria** "Solvation of Coumarine 314 at water/air interfaces containing anionic surfactants. I Low Coverage." Journal of Physical Chemistry B. **109**, 7365 (2005)
- 46 - E. Guardia, J. Marti, L. Garcia Tarres y **D. Laria**.  
"A molecular dynamics simulation study of Hydrogen bonding in aqueous ionic solutions". Journal of Molecular Liquids. **117**, 63, (2005)
- 47 - J. Rodriguez, E. Clavero y **D. Laria**  
"Computer simulations of cationic surfactants adsorbed at air/water interfaces. Journal of Physical Chemistry B, **109**, 24427 (2005)
- 48 - E. Guardia, **D. Laria** y J. Marti  
"Hydrogen bond structure and dynamics in aqueous electrolytes at ambient and supercritical conditions" Journal of Physical Chemistry B. **110**, 6332 (2006)
- 49 - E. Guardia, **D. Laria** y J. Marti

"Reorientational dynamics of water in aqueous ionic solutions at supercritical conditions|: A computer simulation study" Journal of Molecular Liquids, **125**, 107 (2006)

50 – J. Rodriguez y **D. Laria**

"Surface behavior of N-dodecylimidazol at water/air interfaces" Journal of Physical Chemistry C. **111**, 908 (2007)

51– J. Rodriguez, J. Martí, E. Guardia y **D. Laria.**

"Protons in non-ionic aqueous reverse micelles" Journal of Physical Chemistry B **111**, 4432 (2007)

52 – M. Galvagno, **D. Laria** y J. Rodriguez.

"Structural and dynamical characteristics of mesoscopic H<sup>+</sup> H<sub>2</sub>O(n) clusters" Journal of Molecular Liquids, 136, 317 (2007)

53 – E. Clavero, J. Rodriguez y **D. Laria**

"Computer simulations of cationic surfactants adsorbed at air/water interfaces II. Full coverage" Journal of Chemical Physics. **127**, 124704 (2007)

54 - J. Rodriguez, J. Martí, E. Guàrdia y **D. Laria**

"Exploring the picosecond time domain of the solvation dynamics of Coumarin 153 within  $\beta$ -cyclodextrins" Journal of Physical Chemistry B **112**, 8990 (2008)

55 – J. Rodriguez, D. Rico, L. Domenianni y **D. Laria**

"Confinement of polar solvents within  $\beta$ -cyclodextrins" Journal of Physical Chemistry B **112**, 7522 (2008)

56 – M. H. H. Pomata, **D. Laria**, M. S. Skaf y M. D. Elola

"Molecular dynamics simulations of AOT-water/formamide reverse micelles: Structural and dynamical properties". Journal of Chemical Physics **129**, 244503 (2008)

57 - A. C. Furlan, F. W. Fabero, J. Rodriguez, **D. Laria** y M. S. Skaf

"Solvation in supercritical fluids" Publicado en: "Solvation Effects on Molecules and Biomolecules: Computational Methods and Applications". S. Canuto, editor. Páginas: 433-453. Springer, Dordrecht (2008).

58 – J. Rodriguez, R. Semino y **D. Laria**

"Building up Nanotubes: Docking of *Janus* Cyclodextrins in Solutions". Journal of Physical Chemistry B **113**, 1241 (2009)

59 – J. Rodriguez, **D. Laria**, E. Guàrdia y J. Martí

"Dynamics of water nanodroplets and aqueous protons in non-ionic reverse micelles". Physical Chemistry Chemical Physics. **11**, 1484 (2009).

60 – J. Rodriguez, M. D. Elola y **D. Laria**

"Polar mixtures under nanoconfinement" Journal of Physical Chemistry B **113**, 12744 (2009)

61 - J. Rodríguez, M. D. Elola y **D. Laria**

"Coaxial cross-diffusion through carbon nanotubes" Journal of Physical Chemistry B (en prensa)