

RESUME/CV
Luis Guilherme Carvalho Rego

Present Position

Professor

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Research Group

Dynamics of Electrons in Molecules (DynEMol)
website: <http://luisregosites.ufsc.br/>

Research

Our research focuses on the development of nonadiabatic excited-state molecular dynamics and hybrid quantum-classical simulation methods for large scale molecular and mesoscopic systems. Research activities include: the development of theoretical methods for studying charge and energy transfer dynamics in supramolecular systems; the description of coherent electron-phonon and electron-hole dynamics; photoexcitation and charge separation in light-harvesting molecular systems; photoisomerization and mechanisms for quantum control by optical pulses. Some of the physical systems of interest are organic heterostructures, interfaces, dye-sensitized solar cells, transition metal charge-transfer complexes and solvation dynamics. Theoretical formalisms being used include semi-empirical as well as *ab initio* methods.

Education

Ph.D. in Physics: 1993 - 1997

Universidade Estadual de Campinas-UNICAMP (State University of Campinas) &
Institute for Microstructural Sciences, Ottawa, Canada.
Title: *Electronic valence states of SiGe/Si nanostructures*.
Supervisors: Pawel Hawrylak and J.A. Brum.

M.Sc. in Physics: 1990 - 1992,

Universidade Estadual de Campinas-UNICAMP (State University of Campinas).
Title: *Nonequilibrium dynamics of hot carriers and phonons*.

B.S. in Physics: 1986 - 1989,

Universidade de São Paulo-USP (University of Sao Paulo).

Academic Positions

Post-Doctoral Fellow

1997 - 1999.

Department of Physics, Simon Fraser University, BC, Canada. Advisor: George Kirczenow.

2001 - National Synchrotron Light Source Laboratory (LNLS), Brazil. Advisor: Daniel Ugarte.

2002 - Department of Chemistry, Yale University. Advisor: Victor S. Batista.

Teaching

Department of Physics, Universidade Federal de Santa Catarina, Brazil,
2000, 2003 - present.

Main Research Interests

- Theory of nano and mesoscopic systems.
- Excited-State Nonadiabatic Dynamics.
- Electron and energy transport in molecular and solid state systems.
- Development of hybrid Quantum-Classical simulation methods.

List of Selected Recent Publications

Superconducting Qubits as Mechanical Quantum Engines,

Phys. Rev. Lett. **119**, 090601 (2017),

K. Sachtleben, K.T. Mazon, L.G.C. Rego.

featured in Phys.org: <https://phys.org/news/2017-10-superconducting-qubits-function-quantum.html>.

Charge Generation in Organic Solar Cells: Interplay of Quantum Dynamics, Decoherence, and Recombination,

J. Phys. Chem. C, **121**, 23276 (2017)

G. Candiotto, A. Torres, K.T. Mazon, L.G.C. Rego.

A Nonadiabatic Excited State Molecular Mechanics/Extended Hückel Ehrenfest Method,

J. Phys. Chem. C, **120**, 27688 (2016)

R.S. Oliboni, G. Bortolini, A. Torres, L.G.C. Rego.

Vibronic and Coherent Effects on Interfacial Electron Transfer,

J. Phys. Chem. Lett., **6**, 4927 (2015)

R.S. Oliboni, G. Bortolini, A. Torres, L.G.C. Rego.

Surface Effects and Adsorption of Methoxy Anchors on Hybrid Lead Iodide Perovskites: Insights for Spiro-Meotad Attachment,

J. Phys. Chem. C, **118**, 26947 (2014)

A. Torres, L.G.C. Rego.

Intramolecular Polarization Induces Electron-Hole Charge Separation in Light-Harvesting Molecular Triads,

J. Phys. Chem. C, **118**, 126 (2013)

L.G.C. Rego, B. C. Hames, K.T. Mazon, J.O. Joswig.

Influence of Thermal Fluctuations on Interfacial Electron Transfer in Functionalized TiO₂ Semiconductors,

Journal of the American Chemical Society, **127**, 18234 (2005)

S.G. Abuabara, L.G.C. Rego and V.S. Batista.

Quantum Dynamics Simulations of Interfacial Electron Transfer in Sensitized TiO₂ Semiconductors,

Journal of the American Chemical Society, **125**, 7989 (2003)

L.G.C. Rego and V.S. Batista.

Quantized Thermal Conductance of Dielectric Quantum Wires,

Phys. Rev. Lett. **81**, 232 (1998),

L.G.C. Rego and G. Kirczernow.

featured in **Physical Review Focus**: <http://publish.aps.org/FOCUS/v2/st2.html>.

Invited Lectures in International Conferences

American Physical Society Condensed Matter March Meeting

Minneapolis, MN, March 2000,

Title: *A New Principle for Electronic Cooling of Mesoscopic Samples.*

Pan-American Advanced Studies Institute - Physics and Technology at the Nanometer Scale

San Jose, Costa Rica, June 2001

Title: *Thermodynamics of Nanoscopic Systems* - two lectures.

4th J.J. Giambiagi Winter School: Nanophysics, Nanoscience and Nanotechnology

Buenos Aires, Argentina, July 2002

Title: *Heat and charge transport in quasi-1D mesoscopic systems* - two lectures.

36th Winter Colloquium on the Physics of Quantum Electronics

Snowbird, Utah, January 2006

Title: *Coherent Quantum Control of electronic states in functionalized semiconductors.*

253rd American Chemical Society Meeting

San Francisco, CA, April 2017

Title: *Nonadiabatic molecular mechanics/extended Hückel excited state quantum dynamics method.*

Telluride Science Research Center

Telluride, CO, July 2017

Title: *Environmental effects on charge and energy quantum dynamic.*

Personal References

Victor S. Batista:

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George Kirczenow:

Simon Fraser University, BC, Canada
email: kirczeno@sfu.ca

Pawel Hawrylak:

University of Ottawa, Ottawa, CA
email: pawel.hawrylak@uottawa.ca

Daniel Ugarte:

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