CURRICULUM VITAE - Alain Delgado Gran

# 1. PERSONAL DATA

Surnames: Delgado Gran
First and middle names: Alain
Date of birth (Y-M-D): 1975-08-30
Place of Birth: Havana, Cuba.
Nationality: Cuban
Sex: Male
Present Address: 981 Gulf Place K1K 3X9, Ottawa ON, Canada.
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# 2. EDUCATION (Higher Degrees)

- Ph.D. in Physical Sciences (2002-2006): Institute of Cybernetics, Mathematics and Physics (ICIMAF), La Habana, Cuba.
  Title of the Thesis: *"Inelastic Light Scattering by Electronic Excitations in Artificial Atoms"*
  Supervisor: Prof. Dr. Augusto González García.
  Ph.D. degree issued by the National Committee for Scientific Degrees.
  Grade achieved: 5, range [3-5].

- M.Sc. in Physics (1998-2000): Higher Institute of Nuclear Sciences and Technologies (Instec), La Habana, Cuba.
  Title of the Thesis: *"Far-Infrared Giant Dipole Resonances in Neutral Quantum Dots"*
  Supervisor: Prof. Dr. Augusto González García, ICIMAF.
  Co-supervisor: Dr. Roberto Capote Noy, International Atomic Energy Agency (IAEA), Nuclear Data Section, Vienna, Austria.
  M.Sc. degree issued by the Higher Institute of Nuclear Sciences and Technologies.
  Grade achieved: 5, range [3-5].

- B.Sc. in Nuclear Physics (1993-1998): Higher Institute of Nuclear Sciences and Technologies (Instec), La Habana, Cuba.
  Title of the Thesis: *"A Quantum Monte Carlo Approach for Computing the Ground State Energy of Many-Electron Quantum Dots"*
  Supervisor: Prof. Dr. Augusto González García, ICIMAF.
  Co-supervisor: Dr. Roberto Capote Noy, IAEA.
  B.Sc. degree issued by the Higher Institute of Nuclear Sciences and Technologies.
  Grade achieved: 4.86 Summa Cum Laude, range [3-5].

# 3. EMPLOYMENT HISTORY

- (10/2015 - present): Visiting Researcher. Advanced Research Complex, University of Ottawa, Ottawa ON, Canada.
- (10/2012 - 09/2015): Research Associate. S3 Center, NRC Institute of Nanosciences, Modena, Italy.
- (09/2010 - 09/2012): Marie Curie International Incoming Fellow (FP7). S3 Center, NRC Institute of Nanosciences, Modena, Italy.
- (2006 - present): Researcher at the Center of Technical Applications and Nuclear Development, Physics Department, Havana, Cuba.
- Junior associate visits to the Condensed Matter and Statistical Physics Section of the International Centre of Theoretical Physics (ICTP) in Trieste, Italy.
  Periods: (May - August, 2007); (July - October, 2008); (July - October, 2009).
- (2002-2006): Ph.D. Position at the Institute of Cybernetics, Mathematics and Physics (ICIMAF). Condensed Matter Physics Group, Havana, Cuba.
- Three scientific stays (two months each) at the Institute for Microstructural Sciences of the National Research Council of Canada, under the Ph.D. Visiting Student Program.
  2003: Dr. Pawel Hawrylak, Quantum Theory Group.
  2004, 2005: Dr. David J. Lockwood, Optical Spectroscopy of Semiconductor Nanostructures.
- (1998-2002): Young researcher at the Center of Technical Applications and Nuclear Development (CEADEN), Physics Department, Havana, Cuba.

# 4. RESEARCH EXPERIENCE AND SCIENTIFIC INTERESTS

I am a theoretical and computational physicist devoted to the pursuit of knowledge in the fields of condensed matter and quantum chemistry. I have a vast experience in the use of perturbative and non-perturbative many-body methods to model the electronic structure and the optical and dynamical properties of semiconductor nanostructures, molecules and hybrid nanomaterials. My research activity has a strong component of computational physics and chemistry. A more detailed description is given as follows with some references to the list of publications.

### 4.1. Electronic structure calculations and optical properties of hybrid systems with photovoltaic or biological applications .

- Charge-transfer excitations and optical absorption response of metal-organic and pure organic molecular dyes calculated with post-Hartree-Fock electron correlation methods (CI, CAS-SCF,

MRPT) [9] and time-dependent density functional theory (TD-DFT).

- Polarization effects of non-homogeneous and anisotropic dielectric environments (e.g. solvents + semiconductor nanoparticles or surfaces), treated within the Polarizable Continuum Model (PCM), on the opto-electronic and electrochemical properties (ground and excited states oxidation potentials) of molecular dyes used in dye-sensitized solar cells [6].

- *ab initio* real-space DFT and real-time TD-DFT modeling of the coupled electronic and nuclear ultrafast (sub 100 fs) Ehrenfest dynamics of photoexcited states in donor-bridge-acceptor materials engineered for solar energy conversion [4]. I am presently carrying out a new PCM implementation in the code OCTOPUS to model the real-time polarization response of dielectric environments.

### 4.2 Excited states of semiconductor quantum dots.

- Intra- and inter-band excitations spectra of many-electron ( 200 electrons) quantum dots by using the Random Phase (RPA) [19,22] and Configuration Interaction (CI) approximations [13]. Description of collective charge-density (CDE) and spin-density (SDE) excitations.

- Excited states properties under the influence of external electromagnetic fields [15].

- Excitonic and biexcitonic states in many-electron qdots described beyond the mean field approximation by using correlated (CI) wave functions [14,13].

- Excited states of few-electron ($N_e = [2, 6]$) self-assembled quantum dots computed by exact diagonalization of the many-body Hamiltonian [11].

### 4.3 Inelastic Raman scattering by electronic excitations in semiconductor quantum dots.

- Implementation from scratch of a computational methodology to evaluate the second-order electronic Raman cross section in semiconductor quantum dots [19,16,21,15,11] in terms of the many-electron wave functions and energies of the semiconductor nanostructure. The intra- and inter-band electronic states entering the scattering process are described at the level of RPA. Hole states in the valence band are treated within the $4 \times 4$ Kohn-Luttinger formalism.

- The implemented scheme allowed us to investigate theoretically and experimentally a new diapason of physical effects relevant for Raman spectroscopy of quantum dots:

1. the role of electronic correlation and density determined by the lateral confinement potential of the electrons populating the conduction band of the dot. [21].

2. the incident and scattered light polarizations (parallel and crossed) and the electronic Raman selection rules [17].

3. the breakdown of Raman selection rules under the influence of an external magnetic field [15].

4. to set the limits of wide used off-resonance approximation for identifying the charge and spin collective modes in the Raman spectra [17,16].

5. to explore different Laser excitation regimes: below the bandgap, extreme resonance condition and above the bandgap [16,19].

6. the role of the damping of the multielectronic states involved in the scattering process [19].

### 4.4 Coding experience in Condensed Matter Physics and Quantum Chemistry.

- *Experience in the implementation of the following methods of the many-body physics:*

1. Hartree-Fock (HF) method.

2. Density functional theory (DFT).

3. Tamm-Dancoff approximation (TDA).

4. Random Phase Approximation (RPA) and linear response time-dependent DFT (LR-TDDFT).

5. Configuration Interaction (CI).

6. Exact diagonalization techniques using a Lanczos algorithm.

7. Quantum Monte Carlo applied to ground state calculations.

- Most of the methods mentioned above have been efficiently encapsulated in a set Fortran 90 modules which are accessible through the library `Libqdot_01.a(so)` to model electronic the electronic structure and optical processes in semiconductor quantum dots.

- *Experience with atomistic simulation codes:*

- GAMESS (www.msg.chem.iastate.edu/gamess/): user and developer.
- OCTOPUS (www.tddft.org/programs/octopus/wiki/index.php/Main_Page): user and developer.
- NWChem (www.nwchem-sw.org/index.php/Main_Page): user.
- GAUSSIAN (www.gaussian.com/): user.
- ELK (http://elk.sourceforge.net/): basic user.
- CNDOL : user and developer [8].
- Molpro (www.molpro.net/): basic user.

- Development of a code (`NP_BEM.F90`) to solve the Poisson equation for a molecule embedded in an infinite solvent solution and in proximity to a semiconductor nanoparticle (typical configuration found in DSSCs). The polarization response of the dielectric media (solvent and semiconductor nanostructure) is calculated by using the boundary elements method (BEM). This code has been successfully interfaced to GAMESS [6] and is being adapted to work also with OCTOPUS.

- Programing languages: Fortran (object oriented).
- Compilers: gfortran, ifort, pgf90, xlf90.
- HPC Libraries: NETLIB(blas, lapack), Intel MKL, gsl, openMP, openMPI, fft, netcdf, sparskit.
- Bash scripting.

### 4.5 Optical intra-band absorption and dynamical process in microcavity-quantum dot systems.

- Giant Dipole Resonances (GDR) have been traditionally studied in Nuclear Physics. However, it seems to be quite a general phenomenom present in finite systems with two center of charges and we have showed this for the case of neutral (N electron-hole pairs) quantum dots [24,23]. A similar phenomenon can be studied in a microcavity-quantum dot system where exciton-polaritons are formed as a consequence of the coupling of excitons in the qdot with a radiation mode confined in an optical microcavity. The energetic position as well as the intensity of the GDR state is extracted from the calculated first-order correlation function. The GDR physics in this system is investigated in terms of the number of polaritons in the microcavity, the Coulomb interaction strength between carriers in the qdot and the magnitude of the light-matter coupling within the linear response approximation [10].

## 5. SCIENTIFIC COLLABORATIONS

1. Prof. Dr. Guido Goldoni, Dr. Stefano Corni, Dr. Carlo Andrea Rozzi (2010 - ).
   S3 Center, NRC Institute of Nanosciences, Modena, Italy.
   Field(s): First-principles calculations of the electronic and optical properties of hybrid systems with photovoltaic and biological applications; PCM solvation models; *ab-initio* real-space and real-time TD-DFT modeling of the ultrafast dynamics in third-generation photovoltaic devices; Low-dimensional semiconductor nanostructures.

2. Prof. Dr. Angel Rubio (2013 - ).
   Nano-bio spectroscopy group, University of the Basque Country, San Sebastian, Spain.
   Field(s): *ab-initio* real-space and real-time TDDFT modeling of the ultrafast charge transfer dynamics in new materials and molecules of biological interest.

3. Prof. Dr. David J. Lockwood, Principal Research Officer, Surface and Interface Group (2003 - 2009).
   Prof. Dr. Pawel Hawrylak, Group leader, Quantum Theory Group (2003, 2005).
   NRC Institute for Microsctructural Sciences (IMS), Ottawa, Canada.
   Field(s): Electronic Raman scattering of semiconductor quantum dots.

4. Prof. Dr. Luis. A. Montero, Group leader, Quantum Chemistry Laboratory (2008 - 2012).
   Faculty of Chemistry, University of La Habana, Cuba.
   Field(s): Excited states and optical properties of nanoscopic systems; semi-empirical Hamiltonians to study macro-molecules.

5. Dr. Vittorio Pellegrini, Senior Scientist (2007).
   NEST Center, NRC Institute of Nanosciences, Pisa, Italy.
   Field(s): Electronic Raman scattering of many-electron quantum dots under weak confinement regime.

6. Prof. Dr. Eduardo Menendez-Proupín, Associate Professor, Nanomaterials Group (2002, 2009-2013).
   University of Chile, Physics Department, Chile.
   Field(s): *ab-initio* and semi-empirical atomistic models of molecules and nanomaterials; Lifetime of photoexcited sates in quantum dots by considering phononic relaxation mechanisms; Raman scattering in excitonic quantum dots.

7. Prof. Dr. Augusto González (2000 - ).
   Institute of Cybernetics, Mathematics and Physics (ICIMAF), La Habana, Cuba. Field(s): semiconductor quantum dots; electronic structure calculations in atoms and molecules.

8. Dr. Roberto Capote Noy, Nuclear Data Development Unit (2001 - 2006).
   International Atomic Energy Agency (IAEA), Vienna, Austria.
   Field(s): Potential Energy Surface Calculations of Deformed Nuclei; Nuclear structure; Development and optimization of Fortran 90 numerical applications.

# 6. PROJECT COORDINATION/PARTICIPATION

1. **Time dynamics and Control in nanostructures for magnetic recording and energy applications (CRONOS, www.cronostheory.eu)**.

   Duration: 2012 - 2015.
   Total Project budget: EURO 4 441 967
   Budget allocated to S3 Center: EURO 367 363 (solar energy workpackage)
   Financed by: FP7 program of the European Commission.
   Involved Institutions:

   *a*) S3 Center, NRC Institute of nanosciences, Modena, Italy.
   *b*) Trinity College, Dublin, Ireland.
   *c*) Max Planck Society, MPI-Halle, Germany.
   *d*) Fritz Haber Institute, Berlin, Germany.
   *e*) Universidad del Pais Vasco, San Sebastian, Spain.
   *f*) University of Zaragoza, Zaragoza, Spain.
   *g*) Tampere University of Technology, Finland.
   *h*) Universität Oldenburg, Oldenburg, Germany.

*i*) Solaronix SA, Switzerland.

*j*) CNRS-Spintec, France.

Coordinator (S3 Center): Dr. Carlo Andrea Rozzi.
involved researchers (S3 Center): **Dr. Alain Delgado**, Dr. Stefano Pittalis, Dr. Stefano Corni

general objective: to develop a quantitative, flexible and fully atomistic theory of ultrafast dynamics in real materials for advancing two technological areas: solar energy harvesting and ultra-fast and ultra-high density magnetic data storage. CRONOS's theoretical program is experimentally validated by a strong experimental activity on ultrafast pump-probe spectroscopy and industrially validated by the addition to the consortium of the rapidly growing European industry Solaronix.

**2. Optical properties of hybrid organic/inorganic nano-particles for photovoltaic applications: toward a predictive computational approach**.

Duration: 2010 - 2012.
Project budget: EURO 237 272
Financed by: Marie Curie actions, FP7 program of the European Commission.
Involved Institutions:

*a*) S3 Center, NRC Institute of nanosciences, Modena, Italy.

Coordinator: Prof. Dr. Guido Goldoni.
involved researchers: **Dr. Alain Delgado**, Dr. Stefano Corni.

general objective: to build a predictive computational scheme, based on a Configuration Interaction approach, to understand the fundamental mechanisms determining the photoexcitation and charge transfer efficiencies in dye-sensitized solar cells (DSSCs). In a step-by-step strategy toward this goal, we first developed the computational tools to investigate the optical properties of isolated dye molecules by accurate *ab-initio* methods. Then, we have set the theoretical/computational background to model the hybrid system, that is, the dye molecule close to the nanoparticle and embedded in a solvent (electrolyte) solution, and demonstrated the new scheme with a prototype system.

**3. Italian Supercomputing Resource Allocation (ISCRA) projects**

*a*) Class C Project: *"Solvation effects in the optical response and the ultrafast dynamics of organic materials engineered for photovoltaic applications"* (OCT-PCM).
Duration: 11/10/2014 - 11/10/2015.
Project "budget": 1 000 000 cpu hours
Financed by: CINECA supercomputing Center, Bologna, Italy.
HPC Hardware: IBM BG/Q FERMI → 163 840 computing cores.
Involved Institutions: S3 Center, NRC Institute of nanosciences.
Principal investigator: **Dr. Alain Delgado**.
involved researchers: Dr. Carlo Andrea Rozzi, Dr. Stefano Corni, Dr. Stefano Pittalis.

general objective: To model real-time solvation effects in the optical response and the ultrafast charge-transfer dynamics of prototype systems with photovltaic applications by combining the frameworks of TDDFT and the Polarizable Continuum Model (PCM). This project is an important branch of the FP7 European network CRONOS funded under NMP theme.

*b*) Class C Project: *"Charge-transfer excited states and optical response of dye-sensitized solar cells"* (OCT-DSSC).
Duration: 22/03/2013 - 22/03/2014.
Project "budget": 2 000 000 cpu hours
Financed by: CINECA supercomputing Center, Bologna, Italy.
HPC Hardware: IBM BG/Q FERMI → 163 840 computing cores.
Involved Institutions: S3 Center, NRC Institute of nanosciences.
Principal investigator: **Dr. Alain Delgado**.
involved researchers: Dr. Carlo Andrea Rozzi, Dr. Stefano Corni.

general objective: To study the spectrum of electronic excitations and the optical response of $TiO_2$ nanoparticles sensitized with Ruthenium complexes embedded in an acetonitrile solution, within the framework of Time-Dependent Density Functional Theory(TDDFT). The code of choice, OCTOPUS, is capable to apply several kinds of boundary conditions and to include arbitrary time-dependent external fields. The system size ranges up to several hundred atoms and real time runs address the 100 fs time scale, yet evolving at the atto-second rate that characterizes electron dynamics.

*c*) Class B Project: *"Optical properties of metal-organic chromophores in different dielectric environments for photovoltaic applications"* (DEMOOPT).
Duration: 2011 - 2012.
Project "budget": 108 864 cpu hours
Financed by: CINECA supercomputing Center, Bologna, Italy.
HPC Hardware: IBM SP6 → 5376 computing cores.
Involved Institutions: S3 Center, NRC Institute of nanosciences.
Principal investigator: Prof. Dr. Guido Goldoni.
Involved researchers: **Dr. Alain Delgado**, Dr. Stefano Corni.

Main goal: To study the optical properties of selected organic chromophores for photovoltaic (PV) applications in different dielectric environments by *ab-initio* methods. Specifically, in this proposal the optical absorption response and the excited state oxidation potential (ESOP) of selected organic chromophores have been calculated in different dielectric situations of increasing complexity: i) dyes in a homogeneous isotropic solvent; ii) dyes in proximity of a spherical dielectric nanoparticle and in a dielectric solution.

*d*) Class C Project: *"Optical properties of hybrid chromophore/semiconductor nanoparticle systems for photovoltaic applications"* (HY-OPT).

Duration: 2010 - 2011.
Project "budget": 20 000 cpu hours
Financed by: CINECA supercomputing Center, Bologna, Italy.
HPC Hardware: IBM SP6 → 5376 computing cores.
Involved Institutions: S3 Center, NRC Institute of nanosciences.
Principal investigator: Prof. Dr. Guido Goldoni.
Involved researchers: **Dr. Alain Delgado**, Dr. Stefano Corni.

Main goal: to study of the optical properties of an inorganic/organic chromophores use as a realistic dyes in DSSCs. The present proposal served to: i) benchmarking several *ab-initio* quantum-chemistry softwares for the systems of interest; ii) evaluating the suitability of the codes (GAMESS, GAUSSIAN, NWCHEM) for further extensions; iii) calculating the optical excitations of the selected molecular systems. The latter was used for post-processing to include the dielectric effects due to solvent and inorganic nano-particles.

4. **Large Scale Numerical Calculations in Semiconductor Quantum Dots and Biomolecules.**
Duration: 2009 - 2011.
Project budget: CUP 52 622
Financed by: National Program for Developing Basic Sciences in Cuba.
Involved Institutions:

   *a*) Institute of Cybernetics, Mathematics and Physics (ICIMAF), Havana.

   *b*) University of Informatic Sciences (UCI), Havana.

   *c*) Quantum Chemistry Laboratory (QCL), University of Havana.

Coordinator: Prof. Dr. Augusto González (ICIMAF).
Involved researchers: **Dr. Alain Delgado** (ICIMAF): coordinator for designing and implementing the Fortran 90 libraries `libqdot` (optoelectronic properties of qdots) and `libmol` (electronic structure of biomolecules). The aim is to constitute these libraries of well-tested and well-documented pieces of codes that can be used with confidence in all our coding efforts for creating a predictive computational tool. This effort help to avoid duplicated coding work, and facilitate the very important inter-comparisons between existing codes. These computational tools are available to the scientific community working on this subjects such as: different groups at the Faculties of Physics and Chemistry of the University of Havana and the Center of Molecular Immunology of Cuba;
Prof. Dr. Luis. A. Montero (QCL); 3 Ph.D. and 1 M.Sc. students involved.

5. **Inelastic Light Scattering in Semiconductor Quantum Dots.**
Duration: 2006-2008.
Project budget: CUP 54 400
Financed by: National Program for Developing Basic Sciences in Cuba.
Involved Institutions:

   *a*) Institute of Cybernetics, Mathematics and Physics (ICIMAF), Havana.

*b*) Higher Polytechnic Institute, Havana.

*c*) Institute for Microstructural Sciences, National Research Council (IMS-NRC), Canada.

Coordinator: Prof. Dr. Augusto González (ICIMAF).
Involved researchers: **Dr. Alain Delgado** (ICIMAF): Implementation of Configuration Interaction methods and exact diagonalization techniques for computing the spectra of intra- and inter-band excitations of semiconductor quantum dots. Coordinator of the collaboration with the experimental groups of Dr. David J. Lockwood in IMS and Dr. Vittorio Pellegrini in Scuola Normale Superiore of Pisa in charge of performing the experimental measurements of the Raman spectra;
Dr. David J. Lockwood (IMS-NRC); 1 B.Sc. and 1 M.Sc. students involved.

6. **Coordinated Research Program (CRP).**
Duration: 2004-2005.
Project budget: USD 5000
Financed by: International Atomic Energy Agency (IAEA).
Contract officer: Dr. Roberto Capote Noy (IAEA).
Principal investigator: **Dr. Alain Delgado** (ICIMAF): This CRP was carried out in the framework of a major project created during the first research coordination meeting on parameters for calculation of nuclear reactions of relevance to non-energy nuclear applications (Reference Input Parameter Library: Phase III) where a new Fortran 90 modules library MODLIB was developed to be used in existing and future nuclear reaction codes. Specifically, the old Fortran 77 code `om_retrieve.f` for generating the optical model parameters, was encapsulated in a module.

# 7. LANGUAGES

1. Spanish - mother tongue
2. English - Full professional proficiency.
3. Italian - Limited working proficiency.

# 8. TEACHING ACTIVITIES

1. Postgraduate course (conferences and practical sessions) *"Wave Function Based Approximations to Study the Electronic and Optical Properties of Finite Systems"*
Alumni: Ph.D.students at the University of Modena and Reggio-Emilia, Italy, 2015.
2. Postgraduate course (conferences and practical sessions) *"Introduction to the Quantum Mechanics of Many-Particle Finite Systems"*
Alumni: Ph.D. and M.Sc. students at the University of Antioquia, Colombia, 2008.

3. Postgraduate course (practical sessions) *"Quantum Theory of Finite Systems"*
   Alumni: Ph.D. and M.Sc. students at the University of Havana, Cuba, 2007.

4. Postgraduate course (conferences and practical sessions *"Fortran 90 and its Application to Solve Theoretical Physics Problems"*.
   Alumni: M.Sc. and Ph.D. students of the University of Havana and the Institute of Cybernetics, Mathematics and Physics (ICIMAF), La Habana, 2008.

5. Examiner of the B.Sc. Thesis *"Phase Time and Anomalous Effects of Holes Transport in Superlattices"*.
   Author: S. Arias, University of La Habana, 2009.
   Now Ph.D. student at York University, Canada.

6. Examiner of the M.Sc. Thesis *"Dynamical Dissipative Effects in Microcavity - Quantum Dot Systems"*.
   Author: B.Sc. C. Vera, University of Antioquia, Colombia, 2008.
   Now postdoc at University of Wisconsin-Madison, USA.

7. Supervisor of the M.Sc. Thesis *"Excitonic States in Medium-Size Quantum Dots: Beyond the Tamm-Dancoff Approximation"*.
   Author: B.Sc. A. Odriazola, University of La Habana, 2008.
   Now Ph.D. student at Tampere University of Technology, Finland.

8. Supervisor of the B.Sc. Thesis *"Electronic Raman Scattering in Self-Assembled Quantum Dots"*. Author: A. Domínguez (Instec), 2008.
   Now postdoc at University of Bremen, Germany.

# 9. ATTENDED SCIENTIFIC CONFERENCES

1. Octopus developers meeting, Friedrich-Schiller University of Jena, Germany (2015).
   Contribution: Oral presentation; Title: *"A real-space and real-time Polarizable Continuum Model implementation in the Octopus code"*.

2. International workshop *"Solutions for Solvation"*, in honour to Prof. Jacopo Tomasi, Scuola Normale Superiore, Pisa, Italy (2014).

3. Scientific workshop of the European network CRONOS, S3 Center, Institute of Naosciences, Modena, Italy (2014).
   Contribution: Poster; Title: *"Charge separation dynamics and opto-electronic properties of a diaminoterephthalate-$C_{60}$ diad"*.

4. International school and workshop *"6th Time-Dependent Density-Functional Theory: Prospects and Applications"*, Centro de Ciencias de Benasque Pedro Pascual, Spain (2014).

5. International Conference *"Computational Electrostatics for Biological Applications"*, Italian Institute of Technology, Genoa, Italy (2013).
   Contribution: Invited talk; Title: *"Modeling opto-electronic properties of a dye molecule in proximity of a semiconductor nanoparticle"*.

6. CECAM tutorial *"Electronic structure at the cutting edge with Elk"*, CECAM headquarters at the EPFL in Lausanne, Switzerland (2013).

7. International Conference *"62nd Lindau Nobel Laureate Meeting"* dedicated to Physics, Lindau, Germany (2012).

8. International Conference *"Energy from the sun: computational chemist and physicist take up the challenge"*, Sardinia, Italy (2012).
   Contribution: Poster; Title: *"Modeling a dye molecule in the vicinity of a semiconductor nanoparticle"*.

9. International Conference *"Workshop on New Materials for Renewable Energy"*, International Centre for Theoretical Physics (ICTP), Trieste, Italy (2011) .
   Contribution: Poster; Title: *"Low-lying electronic excitations and optical absorption spectra of the black dye sensitizer: a first-principles study"*.

10. International Conference *" Material Science in the Age of Nano"*, Institute of Material Science and Technology (IMRE), La Habana, (2009).
    Contribution: Oral Presentation; Title: *"Computing Electronic and Optical Properties of Quantum Dots"*.

11. International Workshop *"Effective Mass Theoretical Models in Multiband Semiconductor Systems: Applications to Spintronics"*, University of La Habana, (2009).
    Contribution: Invited talk; Title: *"`Libqdot`: A Fortran 90 Module Library for Computing Optical and Electronic Properties of Semiconductor Quantum Dots"*.

12. XI Symposium of the Cuban Physical Society, University of La Habana, Cuba (2008).
    Contribution: 3 poster presentations; Titles: *"Excitonic states in medium-size quantum dots"; "Universality in the Energy Spectrum of medium-Sized Quantum Dots"; " Exact diagonalization studies of inelastic light scattering in self-assembled quantum dots"* .

13. *" Physics of Light-Matter Coupling in Nanostructures"* (PLMCN7), La Habana, Cuba (2007).
    Contribution: 1 oral presentation and 1 poster; Titles: *"Electronic Raman Scattering in Few-Electron Self-Assembled Quantum Dots."; "Theory of Raman Scattering Beyond the RPA in Medium-Size Quantum Dots."*

14. XVII Latin American Symposium on Solid State Physics, La Habana, Cuba (2004).
    Contribution: poster presentation; Title: *"Semiquantitative Theory of Electronic Raman Scattering from Medium-Size Quantum Dots."*

15. *"Quantum Dots 2004"*. Banff, Canada (2004).
    Contribution: poster presentation; Title: *"Resonant Raman Scattering from Quantum Dots."*

16. Theoretical Physics Colloquium in honor to Prof. E. Entralgo. University of La Habana, Cuba (2004).
    Contribution: Invited talk. Title: *"Excited States in Many-Electron Artificial Atoms"*

17. International School on Nano-Science and Nanotechnology. University of La Habana, Cuba (2001).

Contribution: Poster presentation; Title: *"Pygmy Resonances in Artificial Nuclei: Far-Infrared Absorption by Electron-Hole Droplets."*

18. International Workshop *"From Quantum Mechanics to Technology"*. Institute of Cybernetics, Mathematics and Physics (ICIMAF), La Habana, Cuba (2000).
Contribution: oral presentation; Title: *"Far-Infrared Giant Dipole Resonances in Neutral Quantum Dots."*

# 10. INVITED SEMINARS

1. *"Dye-sensitized solar cells from first-principles calculations"*, Quantum Theory Group, Advanced Research Council, University of Ottawa, Canada (2015).

2. *"Modeling solvation effects in real-space and real-time"*, CNR-S3 Center, Institute for Nanoscience, Modena, Italy (2015).

3. *"Modeling opto-electronic properties of a dye molecule in proximity of a semiconductor nanoparticle"*, Institute of Cybernetics, Mathematics and Physics, Centre of Technical Applications and Nuclear Developments, La Habana, Cuba (2013).

4. *"Low-lying electronic excitations and optical absorption spectra of the black dye sensitizer: a first-principles study"*, Institute of Cybernetics, Mathematics and Physics, Centre of Technical Applications and Nuclear Developments, La Habana, Cuba (2011).

5. *"Excited states and optical properties of many and few-electron quantum dots"*, CNR-S3 Center, Institute for Nanoscience, Modena, Italy (2010).

6. *"Configuration Interaction Method Applied to the Study of Many-Electron Quantum Dots"*, Quantum Chemistry Laboratory, University of La Habana (2008); CEADEN, Physics Department, La Habana, Cuba (2008).

7. *"Universality in the Energy Spectrum of Medium-Sized Quantum Dots"*, University of Regensburg, Germany (2008); Atomic and Molecular Physics Department, University of Antioquia, Colombia (2008).

8. *"Electronic Raman Scattering in Semiconductor Quantum Dots"*, University of Leeds, UK (2007); Scuola Normale Superiore, Pisa (2007); University of Regensburg, Germany (2007).

9. *"Spectroscopy of Collective Excitations in Semiconductor Quantum Dots"*, University of La Habana, Department of Theoretical Physics, (2006).

10. *"Breakdown of Electronic Raman Selection Rules in GaAs/AlGaAs Artificial Atoms"*, Nanotalk seminar, IMS-NRC, Canada (2005).

11. *" Excited States of Many-Electron Quantum Dots"*, Quantum Theory Group seminar, IMS-NRC, Canada (2003).

12. *" Resonant Raman Scattering off Neutral Quantum Dots"*, University of La Habana, Cuba (2001).

# 11. SPECIAL RECOGNITIONS

1. Selected as young researcher to participate in the conference "62nd Lindau Nobel Laureate Meeting" dedicated to Physics in Lindau, Germany (2012).
   Nominated by: The Academy of Science for the Developing World (TWAS)
   Supported by: AKB Foundation.

2. Selected as young researcher to participate in the Baden-Württemberg post-conference program of the "62nd Lindau Nobel Laureate Meeting".
   Supported by: Baden-Württemberg Agency for International Economics and Scientific Cooperation.

3. Marie Curie International Incoming Fellowship (MC-IIF).
   Supported by: FP7, Marie Curie Actions. Years: 2010-2012

4. TWAS Fellowship for Research and Advanced Training to carry out a 4 months visit to the Group of Nanomaterials of the University of Chile.
   Supported by:The Academy of Science for the Developing World (TWAS). Year: 2009

5. Referee of the Journals:

   - Physica E: Low Dimensional Systems and Nanostructures.
   - Superlattices and Microstructures.

6. Cuban Academy of Sciences Awards.

   *a*) L.A. Montero, A.L. Montero, C. Bunge, R. Crespo, **A. Delgado**, *et al.*, *"Modeling the optical absorption response of nanoscopic systems"*, 2012.

   *b*) **A. Delgado**, A. Odriazola, A. González, D.J. Lockwood, *"Electronic Raman scattering and electronic excitation spectra of semiconductor quantum dots"*, 2008.

   *c*) A. González, **A. Delgado**, *"Non-perturbative methods in the quantum mechanics of three or more particles"*, 2006.

   *d*) E. Menéndez, C. Trallero-Giner, M. Cardona, S. Ulloa, A. González, **A. Delgado**, *"Raman and hiper-Raman scattering in quantum dot systems"*, 2002.

   *e*) A. González, R. Capote, R. Pérez, B. Rodríguez, **A. Delgado**, E. Menéndez, *"Energy spectrum, density of energy levels, spin polarization and optical properties of quantum dots and atoms traps"*, 2001.

7. Ph.D. Thesis selected by the National Committee for Scientific Degrees in Physics as outstanding Thesis (2006).
   Author: A. Delgado; Supervisor: Prof. Dr. Augusto González.

8. Selected as ICTP Junior Associate of the Condensed Matter and Statistical Physics Section (2005- 2010).

9. Cuban Nuclear Energy Agency Prizes.
   Years: 2015, 2005, 2003, 1999.

10. Graduated Summa Cum Laude of Nuclear Physics (1998).
    Higher Institute of Nuclear Sciences and Technologies (Instec).

# 12. LIST OF PUBLICATIONS

ResearcherID: www.researcherid.com/rid/J-9112-2014

## 12.1. Peer reviewed journals

1. G. Gil, S. Corni, **A. Delgado**, A. Bertoni, G. Goldoni
   *"Excitation energy-transfer in functionalized nanoparticles: going beyond the Förster approach"*
   Journal of Chemical Physics, in press, (2016)
   Publication date: to be defined.

2. **A. Delgado**, S. Corni, S. Pittalis, C.A. Rozzi
   *"Modeling solvation effects in real-space and real-time within Density Functional Approaches"*
   Journal of Chemical Physics 143, 144111 (2015).
   Publication date: 13 October 2015.

3. S. Pittalis, **A. Delgado**, C.A. Rozzi
   *"Same-spin dynamical correlation effects on the electron localization"*
   Journal of Self-Assembly and Molecular Electronics (SAME) 3, 1-14 (2015)
   Publication date: 25 November 2015.

4. Stefano Pittalis, **A. Delgado**, Jörg Robin, Lena Freimuth, Jens Christoffers, Christoph Lienau, Carlo Andrea Rozzi
   *"Charge separation dynamics and opto-electronic properties of a diaminoterephthalate-$C_{60}$ diad"*
   Advanced Functional Materials, DOI: 10.1002/adfm.201402316 .
   Publication date: 10 November 2014.

5. E. Menéndez-Proupin, **A. Delgado**, A. L. Montero-Alejo, J.M. Garca de la Vega
   *"The absorption spectrum of $C_{60}$ in n-hexane solution revisited: fitted experiment and TDDFT/PCM calculations"*
   Chemical Physics Letters 593, 72 (2014).
   Publication date: 6 January 2014.

6. **A. Delgado**, S. Corni, G. Goldoni
   *"Modeling opto-electronic properties of a dye molecule in proximity of a semiconductor nanoparticle"*
   Journal of Chemical Physics 139, 024105 (2013).
   Publication date: 10 July 2013.

7. A. Odriazola, M. M. Ervasti, I. Makkonen, **A. Delgado**, A. González, E. Räsänen, A. Harju
   *"Scaling in the correlation energies of two-dimensional artificial atoms"*
   Journal of Physics: Condensed Matter 25, 505504 (2013).
   Publication date: 25 November 2013.

8. A.L. Montero-Alejo, E. Menndez-Proupin, M.E. Fuentes, **A. Delgado**, F.-P. Montforts, L.A. Montero-Cabrera, J.M. García de la Vega
*"Electronic excitations of $C_{60}$ aggregates"*
Physical Chemistry Chemical Physics 14, 13058 (2012).
Publication date: 19 July 2012.

9. **A. Delgado**, S. Corni, G. Goldoni
*"Low-lying electronic excitations and optical absorption spectra of the black dye sensitizer: a first-principles study"*
Theoretical Chemistry Accounts 131, 1115 (2012).
Publication date: 4 February 2012.

10. Carlos Andres Vera-Ciro, **A. Delgado**, A. González
*"Therahertz Absorption by Excitonic Polaritons"*
Revista Cubana de Física 29, 52 (2012).
Publication date: 3 June 2012.

11. **A. Delgado**, A. Domínguez, R. Pérez, D.J. Lockwood and A. González
*"Exact Diagonalization Studies of Inelastic Light Scattering in Self-Assembled Quantum Dots"*
Physical Review B 79, 195318 (2009).
Publication date: 20 May 2009.

12. A. Odriazola, **A. Delgado**, A. González
*"Propiedades Universales en el Espectro de Energías de Puntos Cuánticos Semiconductores"*
Revista Cubana de Física 26, 61 (2009). *Invited paper.*
Publication date: 18 June 2009.

13. A. Odriazola, **A. Delgado**, A. González
*"Universality in the Energy Spectrum of Medium-Sized Quantum Dots"*
Physical Review B 78, 205320 (2008)
*Also selected by the Virtual Journal of Nanoscale Science and Technology.*
Publication date: 20 November 2008.

14. A. Odriazola, **A. Delgado** and A. González
*"Theory of Excitonic States in Medium-Size Quantum Dots"*
Physical Review B 78, 035329 (2008)
*Also selected by the Virtual Journal of Nanoscale Science and Technology.*
Publication date: 25 July 2008.

15. **A. Delgado**, A. González, D.J. Lockwood
*"Selection and Jump Rules in Electronic Raman Scattering from $GaAs/Al_xGa_{1-x}As$ Artificial Atoms"*
Physical Review B 71, 241311(R) (2005)
*Also selected by the Virtual Journal of Nanoscale Science and Technology.*
Publication date: 24 June 2005.

16. **A. Delgado**, A. Gonzalez, D.J. Lockwood
*"Electronic Raman Scattering in Quantum Dots Revisited"*

Solid State Communications 135, 554 (2005). *Invited paper.*
Publication date: 26 May 2005.

17. A. González, **A. Delgado**
*"Inelastic Light Scattering and the Off-Resonance Approximation"*
Physica E:Low-dimensional Systems and Nanostructures 27, 5 (2005).
Publication date: 8 December 2004.

18. **A. Delgado**, A. González, D.J. Lockwood
*"Dispersión Inelástica de la Luz por Excitaciones Electrónicas en Átomos Artificiales"*
Revista Cubana de Física 22, 142 (2005).

19. **A. Delgado**, A. González and D.J. Lockwood
*"Semiquantitative Theory of Electronic Raman Scattering from Medium-Size Quantum Dots"*
Physical Review B 69, 155314 (2004)
*Also selected by the Virtual Journal of Nanoscale Science and Technology.*
Publication date: 16 April 2004.

20. A. González, **A. Delgado**
*"Resonancia de Ciclotrón y Dispersión Inelástica de Luz en Puntos Cuánticos Semiconductores"*
Revista Cubana de Física 21, 12 (2004).

21. **A. Delgado** and A. González
*"Inelastic Light Scattering and the Excited States of Many-Electron Quantum Dots"*
Journal of Physics: Condensed Matter 15, 4259 (2003).
Publication date: 6 June 2003.

22. **A. Delgado**, A. González and E. Menéndez-Proupín
*"Resonant Raman Scattering off Neutral Quantum Dots"*
Physical Review B 65, 155306 (2002)
*Also selected by the Virtual Journal of Nanoscale Science and Technology.*
Publication date: 26 March 2002.

23. R. Capote, **A. Delgado** and A. González
*"Pygmy Resonances in Artificial Nuclei: Far-Infrared Absorption by Electron-Hole Droplets"*
Modern Physics Letters B 15, 81 (2001).
Publication date: 1 August 2002.

24. **A. Delgado**, L. Lavin, R. Capote and A. Gonzalez
*"Far Infrared Giant Dipole Resonances in Neutral Quantum Dots"*
Physica E:Low-dimensional Systems and Nanostructures 8, 342 (2000).
Publication date: 25 April 2000.

## 12.2. Chapters

1. Stefano Pittalis, **A. Delgado**, Carlo Andrea Rozzi
Chapter 7 *"From reformulations of quantum many-body problems in- and out-of-equilibrium*

*to applications to solar energy conversion on the nanoscale"*
Theory and Applications in Mathematical Physics in Honor of B. Tirozzi's 70th Birthday, 93-106 (2016).

2. L. Lavin, **A. Delgado** and R. Capote
*"Improvements of Pairing Correction for BARRIER Code: Ground State and Saddle Point Deformation of Thorium Isotopes."*
Proceedings of the International Conference "Bologna 2000: Structure of the nucleus at the down of the century", Bologna, Italy, edited by G. Bonsignori, M. Bruno, A. Ventura, D. Vretenar, World Scientific, London, Volume 2 Nuclear Structure, p.249-252 CLAVE: A.