CURRICULUM VITAE - Alain Delgado Gran

1. PERSONAL DATA

Surnames: Delgado Gran

Name: Alain

Date of birth (Y-M-D): 1975-08-30

Place of Birth: Havana, Cuba.

Country of residence: Canada (Permanent Resident) Address: 981 Gulf Place K1K 3X9, Ottawa ON, Canada.

Phone number: +1-(613)-261-5876

e-mail: agran@uottawa.ca

2. EDUCATION (Higher Degrees)

■ Ph.D. in Physical Sciences (2002-2006)

Thesis: "Inelastic Light Scattering by Electronic Excitations in Artificial Atoms"

Supervisor: Prof. Dr. Augusto González.

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

Ph.D. degree issued by the National Committee for Scientific Degrees.

• M.Sc. in Physics (1998-2000)

Thesis: "Far-Infrared Giant Dipole Resonances in Neutral Quantum Dots"

Supervisor: Prof. Dr. Augusto González.

Higher Institute of Nuclear Sciences and Technologies (Instec), Havana, Cuba.

• B.Sc. in Nuclear Physics (1993-1998)

Thesis: "A Quantum Monte Carlo Approach for Computing the Ground State Energy of

Many-Electron Quantum Dots"

Supervisors: Prof. Dr. Augusto González and Dr. Roberto Capote.

Higher Institute of Nuclear Sciences and Technologies (Instec), Havana, Cuba.

3. POSITIONS

- (10/2015 10/2017): Visiting Researcher. Quantum Theory Group, Department of Physics, University of Ottawa, Canada.
- (10/2012 09/2015): Postdoctoral Research Fellow. NRC-Institute of Nanosciences, Modena, Italy.

- (09/2010 09/2012): Marie Curie International Incoming Fellow (FP7). NRC-Institute of Nanosciences, Modena, Italy.
- (2006-2010): Researcher, Condensed Matter Group, Institute of Cybernetics, Mathematics and Physics (ICIMAF), Havana, Cuba.
- Visiting researcher stays, Condensed Matter Physics Section, International Centre of Theoretical Physics (ICTP), Trieste, Italy.
 Periods: (May August, 2007); (July October, 2008); (July October, 2009).
- (2002-2006): Ph.D. fellow, Condensed Matter Group, Institute of Cybernetics, Mathematics and Physics (ICIMAF), 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: Prof. Dr. Pawel Hawrylak, Quantum Theory Group. 2004, 2005: Dr. David J. Lockwood, Optical Spectroscopy of Semiconductor Nanostructures.

• (1998-2016): Researcher, Department of Physics, Centre of Technical Applications and Nuclear Development (CEADEN), Havana, Cuba.

4. RESEARCH EXPERIENCE

I am a theoretical and computational physicist devoted to the pursuit of knowledge in frontier research in material science, condensed matter physics and quantum chemistry. I have focused my scientific efforts on the implementation of quantum theory methods to model and engineer light-matter interaction in nanomaterials, semiconductor nanostructures and hybrid nanodevices with applications in photovoltaics and quantum electronics.

My research activity characterizes by a strong computational component. That is to say, i) extensive use of numerical methods and programing languages at advanced level, ii) developing efficient algorithms for post-processing and visualizing large data sets and iii) expertise in High Performance Computing (HPC) to exploit large-scale computer facilities.

Professional experience and areas of interest:

4.1. Electronic structure calculations and light-matter interactions in 2D materials and semiconductor nanostructures

- 4.1.1) Single-layer and bi-layer Graphene quantum dots in polarizable media.
- 4.1.2) Atomic Si quantum dots in H:Si(100)-2x1 surfaces.
- 4.1.3) 2D Transition Metal Dichalcogenides (TMDCs): band structure, optical properties, spin-orbit and electron-phonon interactions.
 - 4.1.4) Raman (electronic) spectroscopy of collective excitations in nanomaterials.

- 4.1.5) Opto-electronic properties of III-V semiconductor nanostructures.
- 4.1.6) Disordered chains of substitutional dopants in nanocrystals.

4.2. Optical properties and dynamical processes of functionalized materials with photovoltaic applications

- 4.2.1) Excited states calculations and optical response of molecular sensitizers with photovoltaic/biological applications.
- 4.2.2) Charge-transfer and energy-transfer processes mediated in prototypical light-harvesting systems and functionalized carbon-based materials.
- 4.2.3) Extension of the Polarizable Continuum Model (PCM) to address charge and energy transfer events in functionalized materials embedded in non-homogeneous and anisotropic dielectric environments.
- 4.2.4) Modeling of the ultrafast dynamics of photoexcited states in functionalized materials by using real-time TDDFT in conjunction with the Ehrenfest approximation to the nuclei dynamics.

4.3. Methods: quantum theory of many-particle systems

- 4.3.1) Hartree-Fock (HF).
- 4.3.2) Post-HF electron correlation methods
 - a) Tamm-Dancoff approximation (TDA).
 - b) Random phase approximation (RPA).
 - c) Configuration interaction (CI).
 - d) Multi-configuration self-consistent field (MCSCF).
 - e) Multi-reference perturbation theory (MRPT).
- 4.3.3) Density functional approximations
 - a) Kohn-Sham (KS) Density Functional Theory (DFT).
 - b) Time-dependent DFT (TD-DFT) in the time and frequency domains.
- 4.3.4) Exact diagonalization techniques using Lanczos algorithms.
- 4.3.5) Density matrix renormalization group (DMRG).
- 4.3.6) Quantum Monte Carlo applied to ground state calculations.

4.4. Experience with atomistic codes

- 4.4.1) REAL-SPACE AND REAL-TIME REPRESENTATIONS: DFT, TDDFT
 - a) Octopus (www.tddft.org/programs/octopus): developer.
- 4.4.2) PLANE WAVES AND GRIDS: DFT, TDDFT
 - a) Abinit (www.abinit.org): user.

- b) ELK (http://elk.sourceforge.net): user.
- 4.4.3) Tight Binding
- a) QNANO: a computational platform to model atomistically million-atom nanostructures. (http://mysite.science.uottawa.ca/phawrylak/QNANO.html): user and developer.
 - 4.4.4) Gaussian basis sets: wave function methods, DFT, TDDFT
 - a) GAMESS (www.msg.chem.iastate.edu/gamess): user and developer (on a local version).
 - b) NWCHEM (www.nwchem-sw.org/index.php/Main_Page): user.
 - c) GAUSSIAN (www.gaussian.com): user.
 - d) CNDOL: user and developer [14].

4.4.5) NP_BEM

- a) Developed 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). This code has been successfully interfaced to GAMESS [12].
 - 4.4.6) Other technicalities
 - a) Programming languages: Fortran (object oriented (f90-f2003) standards).
 - b) Compilers: gfortran, Intel Fortran, pgf90, xlf90.
 - c) Scientific Libraries: blas, lapack, Intel MKL, gsl, openMP, openMPI, fft, netcdf, sparskit.
 - d) bash scripting.

5. SCIENTIFIC COLLABORATIONS

- 1. Prof. Dr. Guido Goldoni, Dr. Stefano Corni, Dr. Carlo Andrea Rozzi (2010). S3 Center, NRC Institute of Nanosciences, Modena, Italy.
- Prof. Dr. Angel Rubio (2013 2015).
 Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany.
 Nano-bio spectroscopy group, University of the Basque Country, San Sebastian, Spain.
- 3. Prof. Dr. Pawel Hawrylak, Group leader, Quantum Theory Group (2003, 2005). Dr. David J. Lockwood, Principal Research Officer, Surface and Interface Group (2003 2009).
 - NRC Institute for Microsctructural Sciences (IMS), Ottawa, Canada.
- 4. Prof. Dr. Luis. A. Montero, Group leader, Quantum Chemistry Laboratory (2008 2012). Faculty of Chemistry, University of La Habana, Cuba.
- Dr. Vittorio Pellegrini, Senior Scientist (2007).
 NEST Center, NRC Institute of Nanosciences, Pisa, Italy.
- 6. Prof. Dr. Eduardo Menendez-Proupín, Associate Professor, Nanomaterials Group (2002, 2009-2013).
 - University of Chile, Physics Department, Chile.

- 7. Prof. Dr. Augusto González (2000). Institute of Cybernetics, Mathematics and Physics (ICIMAF), La Habana, Cuba.
- 8. Dr. Roberto Capote Noy, Nuclear Data Development Unit (2001 2006). International Atomic Energy Agency (IAEA), Vienna, Austria.

6. PROJECT PARTICIPATION

1. Computational platform for design of atomic scale quantum dot circuits on silicon surface.

Duration: 6 months

Budget allocated to Univ. of Ottawa: CAD (?????)

<u>Financed by:</u> Natural Sciences and Engineering Research Council of Canada (NSERC). <u>Involved Institutions:</u>

- a) Quantum Theory Group, University of Ottawa, Ottawa ON, Canada.
- b) Quantum Silicon Inc., Edmonton, Canada.

Coordinator: Prof. Dr. Pawel Hawrylak

involved researchers: Dr. Alain Delgado, Dr. Marek Korkusinski (NRC)

general objective: The main objective of the proposed project is to develop a new atomistic computational platform, Silicon-QNANO, for the design of atomic scale quantum dot circuits on silicon surface.

2. 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.
- q) 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.

3. 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.

<u>involved researchers:</u> **Dr. Alain Delgado**, Dr. Stefano Corni.

general objective: Building 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).

4. 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).

<u>Duration</u>: 11/10/2014 - 11/10/2015.

Project "budget": 1 000 000 cpu hours

Financed by: CINECA supercomputing Center, Bologna, Italy.

 $\overline{\text{HPC Hardware:}}$ IBM BG/Q FERMI \rightarrow 163 840 computing cores.

 $\underline{\text{Involved Institutions:}}$ S3 Center, NRC Institute of nanosciences.

Principal investigator: Dr. Alain Delgado.

<u>involved researchers:</u> 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).

b) Class C Project: "Charge-transfer excited states and optical response of dye-sensitized solar cells" (OCT-DSSC).

 $\underline{\text{Duration:}}\ 22/03/2013\ -\ 22/03/2014.$

Project "budget": 2 000 000 cpu hours

Financed by: CINECA supercomputing Center, Bologna, Italy.

<u>HPC Hardware:</u> IBM BG/Q FERMI → 163 840 computing cores.

<u>Involved Institutions:</u> S3 Center, NRC Institute of nanosciences.

Principal investigator: Dr. Alain Delgado.

<u>involved researchers:</u> Dr. Carlo Andrea Rozzi, Dr. Stefano Corni.

general objective: To study the spectrum of electronic excitations and the optical response of TiO₂ nanoparticles sensitized with Ruthenium complexes embedded in an acetonitrile solution, within the framework of Time-Dependent Density Functional Theory(TDDFT).

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.

<u>HPC Hardware:</u> IBM SP6 \rightarrow 5376 computing cores.

Involved Institutions: S3 Center, NRC Institute of nanosciences.

Principal investigator: Prof. Dr. Guido Goldoni.

<u>Involved researchers:</u> **Dr. Alain Delgado**, Dr. Stefano Corni.

<u>Main goal:</u> To determine the optical properties of selected organic chromophores for photovoltaic (PV) applications in different dielectric environments by *ab-initio* methods.

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 \rightarrow 5376 computing cores.

<u>Involved Institutions</u>: S3 Center, NRC Institute of nanosciences.

Principal investigator: Prof. Dr. Guido Goldoni.

Involved researchers: Dr. Alain Delgado, Dr. Stefano Corni.

Main goal: Modeling the optical properties of inorganic/organic chromophores used as sensitizers in dye-sensitized solar cells.

5. 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.

<u>Coordinator:</u> Prof. Dr. Augusto González (ICIMAF).

<u>Involved researchers:</u> **Dr. Alain Delgado** (ICIMAF): coordinator for designing and implementing the Fortran 90 libraries libqdot (optoelectronic properties of qdots) and libmol (electronic structure of biomolecules).

Prof. Dr. Luis. A. Montero (QCL); 3 Ph.D. and 1 M.Sc. students involved.

6. 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.

<u>Coordinator:</u> Prof. Dr. Augusto González (ICIMAF).

<u>Involved researchers:</u> **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 performing the experimental Raman spectra.

Dr. David J. Lockwood (IMS-NRC); 1 B.Sc. and 1 M.Sc. students involved.

7. Coordinated Research Program (CRP).

Duration: 2004-2005.

Project budget: USD 5000

Financed by: International Atomic Energy Agency (IAEA).

Contract officer: Dr. Roberto Capote Nov (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.

7. LANGUAGES

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

8. TEACHING ACTIVITIES

1. Two theoretical lectures and hands-on sessions about "ab-initio DFT and TDDFT simulations of finite and extended systems"

Alumni: Undegraduate students at the University of Ottawa, Canada, 2017.

- 2. 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.
- 3. 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.
- 4. Postgraduate course (practical sessions) "Quantum Theory of Finite Systems" Alumni: Ph.D. and M.Sc. students at the University of Havana, Cuba, 2007.
- 5. 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.
- 6. Co-supervisor of Ph.D. student Gabriel Gil Pérez. Project "Electronic excitations in hybrid nanosystems". (2017)

Now Postdoctoral researcher at NRC-Institute of Nanoscience, Modena, Italy.

7. Co-supervisor of Ph.D. student Amintor Dusko during his stay in our group at University of Ottawa in 2016. Project "Effects of disorder in the optical properties of substitutional dopants in Silicon nanocrystals". (2017)

Now postdoctoral fellow at Universidade Federal do Rio de Janeiro, Brasil.

8. 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 postdoctoral fellow at York University, Canada.

9. 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 assistant professor at Universidad de Antioquia, Colombia.

10. 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.

11. Supervisor of the B.Sc. Thesis "Electronic Raman Scattering in Self-Assembled Quantum Dots". Author: A. Domínguez (Instec), 2008.

Now postdoc at Max Planck Institute in Hamburg, Germany.

9. INVITED SEMINARS

- 1. "Modeling Dye-sensitized solar cells from first-principles calculations" Quantum Theory Group (Prof. Dr. Pawel Hawrylak), Department of Physics, University of Ottawa, Canada (2015).
- 2. "Accounting for solvation effects in real-space and real-time TDDFT calculations" NRC-Institute of Nanosciences (Dr. Carlo A. Rozzi), Modena, Italy (2015).
- 3. "Opto-electronic properties of a dye molecule in proximity of a semiconductor nanoparticle"
 - Condensed Matter Group (Prof. Dr. Augusto González), Institute of Cybernetics, Mathematics and Physics (ICIMAF), Havana, Cuba (2013).
- 4. "Low-lying electronic excitations and optical absorption spectra of the black dye sensitizer: a first-principles study"

 Condensed Matter Group (Prof. Dr. Augusto González), Institute of Cybernetics, Mathematics and Physics (ICIMAF), Havana, Cuba (2011).
- 5. "Excited states and optical properties of many-electron quantum dots" NRC-Institute of Nanosciences (Prof. Dr. Elisa Molinari), Modena, Italy (2010).
- 6. "Configuration interaction method applied to the study of many-electron quantum dots" Quantum Chemistry Lab (Prof. Dr. Luis A. Montero), University of Havana, Cuba (2008).
- 7. "Universality in the energy spectrum of medium-sized quantum dots" Group of Optical Spectroscopy of Semiconductor Quantum Structures (Prof. Dr. Christian Schüller) University of Regensburg, Germany (2008)
- 8. "Theory of excitonic states in medium-sized quantum dots"

 Department of Physics (Prof. Dr. Boris Rodríguez), University of Antioquia, Medellín,
 Colombia (2008).
- 9. "Spectroscopy of collective excitations in semiconductor quantum dots" Group of Optical Spectroscopy of Semiconductor Quantum Structures (Prof. Dr. Christian Schüller) University of Regensburg, Germany (2007)
- "Electronic Raman scattering in semiconductor quantum dots"
 Institute of Microwave and Photonics (Prof. Dr. Paul Harrison), University of Leeds, UK (2007).
 Scuola Normale Superiore (Prof. Dr. Vittorio Pellegrini), Pisa, Italy (2007).
- 11. "Selection and jump rules in electronic Raman scattering from GaAs/AlGaAs artificial atoms"

 Quantum Theory Group (Prof. Dr. Pawel Hawrylak), NRC-Institute for Microstructural Sciences, Ottawa, Canada (2005).
- 12. "Excited states of many-electron quantum dots" Quantum Theory Group (Prof. Dr. Pawel Hawrylak), NRC-Institute for Microstructural Sciences, Ottawa, Canada (2003).

13. "Resonant Raman scattering off neutral quantum dots"

Department of Physics (Prof. Dr. Carlos Trallero-Giner), University of Havana, Cuba (2001).

10. SCIENTIFIC CONFERENCES

- 1. 2017 High Performance Computing Symposium, Queens University, Kingston, Canada (2017).
 - Contribution: Invited talk; <u>Title:</u> "Electronic and optical properties of molecules and graphene and semiconductor quantum dots computational tools".
- 2. Solvation, non-uniform polarizability, and local field effects in solids, liquids, life, and devices, University of British Columbia, Vancouver, Canada (2016).

 <u>Contribution: Invited talk; Title: "Abinitio modeling of optoelectronic properties of polyatomic molecules in solvents and in proximity to a semiconductor nanoparticle".</u>
- 3. Theory Canada 11, University of Carleton, Ottawa, Canada (2016).

 <u>Contribution: Oral presentation; Title:</u> "Modeling solvation effects in real-space and real-time within Density Functional Approaches".
- 4. Octopus developers meeting, Friedrich-Schiller University of Jena, Germany (2015).

 <u>Contribution: Oral presentation; Title:</u> "A real-space and real-time Polarizable Continuum Model implementation in the Octopus code".
- 5. International workshop "Solutions for Solvation", in honour to Prof. Jacopo Tomasi, Scuola Normale Superiore, Pisa, Italy (2014).
- Scientific workshop of the European network CRONOS, S3 Center, Institute of Naosciences, Modena, Italy (2014).
 Contribution: Poster; <u>Title:</u> "Charge separation dynamics and opto-electronic properties of a diaminoterephthalate-C₆₀ diad".
- 7. International school and workshop "6th Time-Dependent Density-Functional Theory: Prospects and Applications", Centro de Ciencias de Benasque Pedro Pascual, Spain (2014).
- 8. International Conference "Computational Electrostatics for Biological Applications", Italian Institute of Technology, Genoa, Italy (2013).

 <u>Contribution:</u> Invited talk; <u>Title:</u> "Modeling opto-electronic properties of a dye molecule in proximity of a semiconductor nanoparticle".
- 9. CECAM tutorial "Electronic structure at the cutting edge with Elk", CECAM headquarters at the EPFL in Lausanne, Switzerland (2013).
- 10. International Conference "62nd Lindau Nobel Laureate Meeting" dedicated to Physics, Lindau, Germany (2012).
- 11. 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".

- 12. International Conference "Workshop on New Materials for Renewable Energy", International Centre for Theoretical Physics (ICTP), Trieste, Italy (2011).

 <u>Contribution:</u> Poster; <u>Title:</u> "Low-lying electronic excitations and optical absorption spectra of the black dye sensitizer: a first-principles study".
- 13. International Conference "Material Science in the Age of Nano", Institute of Material Science and Technology (IMRE), La Habana, (2009).

 <u>Contribution:</u> Oral Presentation; <u>Title:</u> "Computing Electronic and Optical Properties of Quantum Dots".
- 14. 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".
- 15. XI Symposium of the Cuban Physical Society, University of La Habana, Cuba (2008).

 <u>Contribution:</u> 3 poster presentations; <u>Titles:</u> "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".
- 16. "Physics of Light-Matter Coupling in Nanostructures" (PLMCN7), La Habana, Cuba (2007).
 Contribution: 1 oral presentation and 1 poster; <u>Titles:</u> "Electronic Raman Scattering in Few-Electron Self-Assembled Quantum Dots."; "Theory of Raman Scattering Beyond the RPA in Medium-Size Quantum Dots."
- 17. XVII Latin American Symposium on Solid State Physics, La Habana, Cuba (2004).

 <u>Contribution:</u> poster presentation; <u>Title:</u> "Semiquantitative Theory of Electronic Raman Scattering from Medium-Size Quantum Dots."
- 18. "Quantum Dots 2004". Banff, Canada (2004).

 <u>Contribution:</u> poster presentation; <u>Title:</u> "Resonant Raman Scattering from Quantum Dots."
- 19. Theoretical Physics Colloquium in honor to Prof. E. Entralgo. University of La Habana, Cuba (2004).

 <u>Contribution:</u> Invited talk. <u>Title:</u> "Excited States in Many-Electron Artificial Atoms"
- International School on Nano-Science and Nanotechnology. University of La Habana, Cuba (2001).
 Contribution: Poster presentation; <u>Title:</u> "Pygmy Resonances in Artificial Nuclei: Far-Infrared Absorption by Electron-Hole Droplets."
- 21. International Workshop "From Quantum Mechanics to Technology". Institute of Cybernetics, Mathematics and Physics (ICIMAF), La Habana, Cuba (2000).

 <u>Contribution:</u> oral presentation; <u>Title:</u> "Far-Infrared Giant Dipole Resonances in Neutral Quantum Dots."

11. DISTINCTIONS/AWARDS

- Selected as young researcher to participate in the 62nd Lindau Nobel Laureate Meeting dedicated to Physics, Lindau, Germany (2012).
 Nominated by: The World Academy of Sciences (TWAS)
- 2. Selected as young researcher to engage 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: Marie Curie Actions, European Comission. Years: 2010-2012
- 4. Ph.D. Thesis selected by the National Committee for Scientific Degrees in Physics as outstanding thesis in 2006.
- 5. Associate member of the Condensed Matter and Statistical Physics Section of the International Centre for Theoretical Physics (ICTP, Trieste, Italy) for the period 2005-2010.
- 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. TWAS Fellowship for Research and Advanced Training in 2009. Supported by:The Academy of Science for the Developing World (TWAS).
- 8. Cuban Nuclear Energy Agency Prizes. Years: 2015, 2005, 2003, 1999.
- 9. Graduated Summa Cum Laude of Nuclear Physics (1998). Higher Institute of Nuclear Sciences and Technologies (Instec).

12. PEER REVIEW ACTIVITY

• Physica E: Low Dimensional Systems and Nanostructures.

- Superlattices and Microstructures.
- Journal of Chemical Physics.
- Computational and Theoretical Chemistry.

13. PUBLICATIONS

Scientific production is supported by 28 articles published in peer-review journals and 2 book chapters. More details can be consulted in my researcherID page: www.researcherid.com/rid/J-9112-2014

13.1. Peer reviewed journals

- 1. **A. Delgado**, M. Korkusinski, P. Hawrylak "Atomic quantum dots in H-Si(100)-2x1 surfaces" Article to be submitted to Physical Review B
- 2. Y. Saleem, L. Nagera, **A. Delgado**, L. Szulakowska, P. Hawrylak "Band gaps and optical properties of hexagonal graphene quantum dots of increasing sizes" Article to be submitted to Physical Review B
- 3. Amintor Dusko, **A. Delgado**, Andrei Saraiva, Belita Koiller "Adequacy of Si:P Chains as Fermi-Hubbard Simulators" Submitted to Nature Partner Journals Quantum Information (NPJQI-00321)
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