

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.

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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 -): Research scientist. 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. DISTINCTIONS/AWARDS

1. 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 Commission. 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).

5. 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.

5.1. 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)
10. “*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).

5.2. INVITED TALKS

1. 2017 High Performance Computing Symposium (HPCS2017), Queens University, Kingston, Canada (2017).
Title: “*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).
Title: “*Abinitio modeling of optoelectronic properties of polyatomic molecules in solvents and in proximity to a semiconductor nanoparticle*”.

3. Theory Canada 11, University of Carleton, Ottawa, Canada (2016).
Title: “*Modeling solvation effects in real-space and real-time within Density Functional Approaches*”.
4. Octopus developers meeting, Friedrich-Schiller University of Jena, Germany (2015).
Title: “*A real-space and real-time Polarizable Continuum Model implementation in the Octopus code*”.
5. International Conference “*Computational Electrostatics for Biological Applications*”, Italian Institute of Technology, Genoa, Italy (2013).
Title: “*Modeling opto-electronic properties of a dye molecule in proximity of a semiconductor nanoparticle*”.
6. International Conference “*Material Science in the Age of Nano*”, Institute of Material Science and Technology (IMRE), Havana (2009).
Title: “*Computing Electronic and Optical Properties of Quantum Dots*”.
7. International Workshop “*Effective Mass Theoretical Models in Multiband Semiconductor Systems: Applications to Spintronics*”, University of Havana (2009).
Title: “*Libqdot: A Fortran 90 Module Library for Computing Optical and Electronic Properties of Semiconductor Many-Electron Quantum Dots*”.
8. “*Physics of Light-Matter Coupling in Nanostructures*” (PLMCN7), Havana Cuba (2007).
Titles: “*Electronic Raman Scattering in Few-Electron Self-Assembled Quantum Dots.*”; “*Theory of Raman Scattering Beyond the RPA in Medium-Size Quantum Dots.*”
9. Theoretical Physics Colloquium in honor to Prof. E. Entralgo. University of La Habana, Cuba (2004).
Title: “*Excited States in Many-Electron Artificial Atoms*”
10. International Workshop “*From Quantum Mechanics to Technology*”. Institute of Cybernetics, Mathematics and Physics (ICIMAF), La Habana, Cuba (2000).
Title: “*Far-Infrared Giant Dipole Resonances in Neutral Quantum Dots.*”

5.3. PUBLICATIONS

Scientific production is supported by 30 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

5.3.1. 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"
 npj Quantum Information, doi:10.1038/s41534-017-0051-1 (2018)
 Publication date: 10 January 2018.
4. J. Jadczak, **A. Delgado**, L. Bryja, Y. S. Huang, P. Hawrylak
"Robust high-temperature trions emission in monolayers of $\text{Mo}(\text{S}_y\text{Se}_{1-y})_2$ alloys"
 Physical Review B 95, 195427 (2017)
5. S. Pittalis, D. Varsano, **A. Delgado**, C.A. Rozzi
"Probing electron localization by means of coalescent pairs: A simple DFT-based approach"
 Invited paper: special issue of European Physics Journal in Honor to Hardy Gross 2017
6. G. Gil, S. Corni, **A. Delgado**, A. Bertoni, G. Goldoni
"Predicting signatures of anisotropic resonance energy transfer in dye-functionalized nanoparticles"
 RSC Advances 6, 104648 (2016)
 Publication date: 25 October 2016.
7. 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 144, 074101 (2016)
 Publication date: 16 February 2016.
8. 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.
9. **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.
10. 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 25, 2047 (2015) .
 Publication date: 10 November 2014.
11. 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.

12. **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.
13. 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.
14. A.L. Montero-Alejo, E. Menéndez-Proupin, M.E. Fuentes, **A. Delgado**, F.-P. Montforts, L.A. Montero-Cabrera, J.M. García de la Vega
"Electronic excitations of C₆₀ aggregates"
 Physical Chemistry Chemical Physics 14, 13058 (2012).
 Publication date: 19 July 2012.
15. **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.
16. Carlos Andres Vera-Ciro, **A. Delgado**, A. González
"Terahertz Absorption by Excitonic Polaritons"
 Revista Cubana de Física 29, 52 (2012).
 Publication date: 3 June 2012.
17. **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.
18. 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.
19. 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.
20. 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.

21. **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.
22. **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.
23. 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.
24. **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).
25. **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.
26. A. González, **A. Delgado**
"Resonancia de Ciclotrón y Dispersión Inelástica de Luz en Puntos Cuánticos Semiconductores"
Revista Cubana de Física 21, 12 (2004).
27. **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.
28. **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.
29. 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.

30. **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.

5.3.2. Book 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 dawn 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.