

Curriculum Vitae

Andrés Reyes

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Date and place of birth: March 11, 1974 in Cali, Colombia

I EDUCATION

- 1997 B.Sc. in Chemistry, Universidad del Valle, Colombia
2003 Ph.D. in Chemistry, University of Florida, USA

II PROFESSIONAL EXPERIENCE

- 2003-2005 Postdoctoral Fellow, Department of Chemistry, Penn State University, USA
2005-2013 Associate Professor of Chemistry, Universidad Nacional de Colombia, Bogotá, Colombia
2013-2014 Visiting Professor, Institute of Physics, University of Sao Paulo, Sao Paulo, Brazil
2013-present Professor of Chemistry, Universidad Nacional de Colombia, Bogotá, Colombia

III HONORS and AWARDS

- 2002 Delores A. Auzenne Fellowship, University of Florida, USA
2003 Chemical Physics Certificate, University of Florida, USA
2008 Wiley Young Investigator Award, Sanibel Symposium, USA

IV PROFESSIONAL SERVICE

- 2008 Organizer: 2nd Colombian Theoretical and Computational Chemists Meeting, 2008, Calarcá, Colombia
2009 Organizer: 35th Congress of Theoretical Chemists of Latin Expression, QUITEL 2009, San Andrés, Colombia
2011 Co-organizer: Pan American Advances Institute: Electronic Properties of Complex Systems, 2011, Cartagena, Colombia

V SUPERVISED COLLABORATORS

v.1 Current research group

Ph. D. students: Mauricio Rodas, Edwin Posada, Rubén Dario Guerrero, Ismael Ortiz

Masters students: Matheus Rodríguez, Ronald González, Jorge Charry, Alejandro Peña, Danilo González, Laura Pedraza

Undergraduate students: Carlos Ortiz

Postdoctoral scholar: Johan Galindo

v.2 Former members

Posdoctoral scholars

Dr. Hugo Bohórquez, 2011-2012.

Current position: Researcher, Instituto Inmunológico, Bogotá, Colombia

Master of Science

Néstor Aguirre, MSc, 2008. Summa cum laude.

Current position: Postdoctoral Fellow in Chemistry, Universidad Autónoma, Madrid, Spain

Ismael Ortiz, MSc, 2009

Current position: Doctoral student in Chemistry, Universidad Nacional de Colombia

Sergio González, MSc, 2010. Summa cum laude.

Current position: Instituto Nacional de Metrología

Diego Moreno, MSc, 2010.

Current position: Doctoral student in Chemistry, Universidad de Guanajuato, Guanajuato, Mexico

Edwin Posada, MSc, 2011.

Current position: Doctoral student in Chemistry, Universidad Nacional de Colombia

Neftalí Forero, MSc, 2013

Jonathan Romero, MSc, 2014. Summa cum laude.

Current position: Doctoral student in Chemistry, Harvard University, USA

Felix Moncada, MSc, 2014. Summa cum laude.

Current position: Lecturer, Universidad de la Amazonia, Florencia, Colombia

Undergraduate students: Sergio González (B.Sc. 2008), Neftalí Forero (B.Sc. 2009), Jonathan Romero (B.Sc. 2011), Felix Moncada (B.Sc. 2011), Lalita Uribe (B.Sc. 2011), Jorge Charry (B.Sc. 2012), Alejandro Peña (B.Sc. 2013)

VI RESEARCH GRANTS (2009-)

Research Office, Universidad Nacional, Bogota Fund for research groups supporting graduate programs	2014-2015	30.000.000 COP
Research Office, Universidad Nacional, Bogota Fund for research groups supporting graduate programs	2014-2015	30.000.000 COP
Research Office, Universidad Nacional, Bogota Fund for research groups supporting graduate programs	2012-2013	60.000.000 COP
Research Office, Universidad Nacional, Bogota Theoretical development and computational implementation in CUDA of the Herman-Kluk and its application for the determination of molecular rotational spectra	2012-2013	40.000.000 COP
Research Office, Universidad Nacional, Bogota LOWDIN: a computational code to study electron and nuclear structure	2011-2013	60.000.000 COP
Research Office, Universidad Nacional, Bogota Theoretical development and computational implementation of the nuclear propagator method and its application in chemistry	2010-2012	40.000.000 COP
Research Office, Universidad Nacional, Bogota Endohedral fullerenes: Theoretical study of their structures	2010-2012	40.000.000 COP
COLCIENCIAS Dynamics, spectroscopy and solvent effects of the transition state of halogen reactions $X+HY \rightarrow XH + Y$. In collaboration with Prof. José Lopez, Universidad del Valle, Colombia	2010-2012	162.122.000 COP
COLCIENCIAS (Colombia-Mexico) Isotope effects in Hydrogen Bonding. In collaboration with Prof. Gabriel Merino, Universidad de Guanajuato, Mexico	2009-2011	17.400.000 COP
COLCIENCIAS (Colombia-Spain) Nuclear quantum effects in hydrogen bonding and its application to water clusters. In collaboration with Dr. María de Lara, CSIC Madrid, Spain	2010-2012	19.000.000 COP
Research Office, Universidad Nacional, Bogota Nuclear quantum effects in water dimer isotopomers	2009-2010	40.000.000 COP
COLCIENCIAS First principles study of giant isotope effects in $K_3H(SO_4)_2$	2009-2011	94.200.000 COP
Research Office, Universidad Nacional, Bogota Implementation of the MP2-RI method in the APMO code. In collaboration with Prof. Roberto Flores, Universidad de Guadalajara, Mexico	2009-2010	10.000.000 COP
Research Office, Universidad Nacional, Bogota First principles study of kinetic isotope effects	2008-2009	30.000.000 COP

VII INVITED TALKS (2010-)

1. *Calculation of binding energies using the Any Particl Molecular Orbital approach*, Encontro Nacional de Física da Materia Condensada, May 2014, Costa Sauipe, Brazil
2. *Calculation of Any Particle Binding Energies with the Generalized Any Particle Propagator Method*, XVIII Workshop on Quantum Systems in Chemistry, Physics and Biology, December 2013, Paraty, Brazil
3. *Muonic Alchemy: Transmuting elements one muon at a time*, Colloquium of the Physics Institute, University of Sao Paulo, November 2013, Sao Paulo, Brazil
4. *Atomic Contributions to the Rotational Barrier of Biphenyl*, Físico Química en América Latina, October 2013, Foz de Iguazú, Brazil
5. *Transmuting elements one muon at a time*, IV SEEDMOL Symposium, September 2012, Piranópolis, Brazil
6. *Structure and properties of atoms and molecules confined inside fullerenes*, 7th International Meeting on Photodynamics and Related Aspects, October 2012, Maresias, Brazil
7. *Transmutando átomos un muón a la vez*, I Escuela Colombiana de Teoría y Computación en las Ciencias Moleculares, April 2012, Cali, Colombia
8. *Muon Alchemy: transmuting elements with the inclusion of negative muons*, 37th Congress of Theoretical Chemists of Latin Expression, December 2011, Rivera Maya, Mexico
9. *Chemistry beyond the Born-Oppenheimer Approximation*, 10 Simposio Día de la Química, November 2011, Manizalez, Colombia
10. *A theoretical study of the quantum state of atoms trapped inside fullerenes*, 9th WATOC congress, July 2011, Santiago de Compostela, Spain
11. *Nuclear mass and delocalization effects in chemistry*, Chemistry Department, University of Buenos Aires, December 2010, Buenos Aires, Argentina
12. *Nuclear mass and delocalization effects in quantum chemistry*, III CFQTC, December 2010, Caracas, Venezuela
13. *Nuclear mass and delocalization effects in quantum chemistry*, III SEEDMOL, October 2010, Brasilia, Brazil
14. *Nuclear quantum effects in quantum chemistry*, 36th Congress of Theoretical Chemists of Latin Expression, September 2010, Anglet, France
15. *Nuclear quantum effects on molecular structure*, 12eme Rencontre des Chimistes Théoriciens Francophones, July 2010, Namur, Belgium
16. *Nuclear quantum effects on molecular structure*, Chemistry Department, Universidad de Guanajuato, May 2010, Guanajuato, Mexico
17. *Nuclear quantum effects on molecular structure*, Chemistry Department, Universidad de Guadalajara, May 2010, Guadalajara, Mexico

VIII POSTER CONTRIBUTIONS (2008-)

1. J. Romero, M. Diaz Tinoco, J. V. Ortiz, R. Flores Moreno, A. Reyes, *A generalized any particle propagator: prediction of proton affinities and acidity properties with the H⁺ propagator*, 53rd Sanibel Symposium, St Simons Island, Georgia, USA, 2013
2. J. Charry, F. Moncada, E. Posada, J. Romero, A. Reyes, *Structure and properties of atoms and molecules conned inside fullerenes*, 53rd Sanibel Symposium, St Simons Island, Georgia, USA, 2013
3. R. D. Guerrero, C. A. Arango, A. Reyes, *Optimal Control of Wave-Packets: a Semiclassical Approach*, 53rd Sanibel Symposium, St Simons Island, Georgia, USA, 2013
4. R. D. Guerrero, C. A. Arango, A. Reyes, *Semiclassical Optimal Control of Wave-Packets: an Application to Diatomic Rotors in Tilted Fields*, 7th International Meeting on Photodynamics, Maresias, Brasil, 2012
5. F. Moncada, D. Cruz, A. Reyes, *Muon Alchemy: transmuting elements with the inclusion of negative muons*, 52nd Sanibel Symposium, St Simons Island, Georgia, USA, 2012
6. J. Romero, R. Flores-Moreno, A. Reyes, *Any particle binding energy calculations using propagator theory*, 52nd Sanibel Symposium, St Simons Island, Georgia, USA, 2012
7. F. Moncada, J. Romero, A. Reyes *A quantum description of ³He_n (n=1,2) atoms confined in C₆₀*, 52nd Sanibel Symposium, St Simons Island, Georgia, USA, 2012
8. J. Charry, A. Reyes, *Implementation of the Colle-Salvetti functional for nuclear-electronic correlation*, 37th Congress of Theoretical Chemists of Latin Expression, Riviera Maya, Mexico, December 2011
9. J. M. Rodas, A. Reyes, *Nuclear quantum effects on symmetric and assymetric intramolecular hydrogen bonds*, 37th Congress of Theoretical Chemists of Latin Expression, Riviera Maya, Mexico, December 2011
10. J. Romero, R. Flores-Moreno, A. Reyes, *Propagator theory applied to electrons and nuclei*, 37th Congress of Theoretical Chemists of Latin Expression, Riviera Maya, Mexico, December 2011
11. F. Moncada, A. Reyes, R. Flores-Moreno, *Theoretical study of isotope effects in polarizabilities*, 37th Congress of Theoretical Chemists of Latin Expression, Riviera Maya, Mexico, December 2011
12. R. Guerrero, C. A. Arango, A. Reyes, *Semiclassical optimal control of the coherent wave-packet of a molecular rotor*, 37th Congress of Theoretical Chemists of Latin Expression, Riviera Maya, Mexico, December 2011
13. H. J. Bohorquez and A. Reyes, *Local quantum chemistry*, 37th Congress of Theoretical Chemists of Latin Expression, Riviera Maya, Mexico, December 2011
14. J. Romero, R. Flores-Moreno, A. Reyes, *Theoretical study of isotope effects on electron ionization using propagator theory*, 9th WATOC conference, Santiago de Compostela, España. July 2011

15. F. Moncada, A. Reyes, Roberto Flores-Moreno, *Theoretical study of isotope effects in photo-electron spectroscopy*, 9th WATOC, Santiago de Compostela, España July, 2011
16. J. Romero, R. Flores-Moreno, A. Reyes, *Theoretical study of isotope effects on electron ionization using propagator theory*, Pan American Advanced Studies Institute. Cartagena, Colombia. June, 2011
17. F. Moncada, A. Reyes, R. Flores-Moreno, *Localized Hartree products as nuclear wavefunctions*, Pan American Advanced Studies Institute (PASI) in electronic properties of complex systems, Cartagena, Colombia June, 2011
18. F. Moncada, S. A González, A. Reyes, *First principles investigation of hydrogen isotope effects in [XSO₄-H-SO₄X]- (X = H,K) complexes*, 50th Sanibel Symposium, St Simons Island, Georgia, USA, 2010
19. D. Moreno, S. A. González, A. Reyes, *Nuclear quantum effects on low barrier hydrogen bonds*, 49th Sanibel Symposium, St. Simons Island, USA, 2009
20. S. A. González, A. Reyes, *Theoretical investigation of hydrogen isotope effects in water dimers*, 49th Sanibel Symposium, St. Simons Island, USA, 2009
21. J. Galindo, S. A. González, A. Reyes, *Theoretical investigation of positronic molecules*, 49th Sanibel Symposium, St. Simons Island, USA, 2009
22. S. A González, A. Reyes, *Investigation of isotope effects with the APMO code*, 13th International Symposium of Quantum Chemistry, Helsinki, Finland, 2009
23. N. Forero, S. A González, A. Reyes, *Efecto isotópico de hidrógeno en complejos donor-aceptor mediante el uso de orbitales moleculares nucleares*, 35th Congress of Theoretical Chemists of Latin Expression, San Andrés, Colombia, 2009
24. F. Moncada, S. A González, A. Reyes, *First principles study of the isotope effect on the phase temperature of K₃H(SO₄)₂ and K₃D(SO₄)₂*, 35th Congress of Theoretical Chemists of Latin Expression, San Andrés, Colombia, 2009
25. D. Moreno, S. A González, A. Reyes, *Estudio del efecto de isótopo de hidrógeno en la estabilidad de complejos oleofina: X+ (X: Li, Na, K)*, 35th Congress of Theoretical Chemists of Latin Expression, San Andrés, Colombia, 2009
26. J. Romero, S. A González, A. Reyes, *Secondary hydrogen isotope effects on the acidity as calculated with the APMO code*, 35th Congress of Theoretical Chemists of Latin Expression, San Andrés, Colombia, 2009
27. I. Ortiz, S. A González, A. Reyes, *Estudio del efecto isotópico de hidrógeno en sistemas unidos por puentes de dihidrógeno*, 35th Congress of Theoretical Chemists of Latin Expression, San Andrés, Colombia, 2009
28. S. A. González, N. F. Aguirre, A. Reyes, *Investigation of isotope effects from first principles*, GRC on Isotopes in Biological and Chemical Sciences, Ventura, USA, 2008
29. S. A. González, N. F. Aguirre, A. Reyes, *Investigation of isotope effects from first principles*, 48th Sanibel Symposium, St. Simons Island, USA, 2008

IX PUBLICATION

IX.1 Submitted

1. E. Posada, F. Moncada, A. Reyes, *Disentangling the quantum muon and nuclear mass effects in negative muonic atoms*, J. Phys. Chem. A, Submitted (2014)
2. J. Romero, J. Charry, R. Flores-Moreno, M. Varella, A. Reyes, *Calculation of positron binding energies using the generalized any particle propagator theory*, J. Chem. Phys., Accepted (2014)

IX.2 Published

1. J. Charry, J. Romero, M. Varella, A. Reyes, *Positron binding energies of amino acids with the generalized any-particle propagator method*, Phys. Rev. A, **89** 052709 (2014)
2. S. Pan, D. Moreno, J. L. Cabellos, J. Romero, A. Reyes, G. Merino, P. K. Chattaraj, *In Quest of Strong Be-Ng Bonds Among the Neutral Ng-Be Complexes*, J. Phys. Chem. A, **118** 487 (2014)
3. H. J. Bohórquez, A. Reyes, *The atomic Pauli energy grows exponentially with the electronic localization*, Mol. Phys., **112** 416 (2014)
4. J. Romero, A. Restrepo, A. Reyes, *Solvent isotope effects on the hydration of alkaline cations: H/D secondary isotope effects on electrostatic interactions*, Mol. Phys., **112** 518 (2014)
5. R. D. Guerrero, C. A. Arango, A. Reyes, *Semiclassical optimal control of wave-packets: an application to diatomic rotors in tilted fields*, Mol. Phys., **112** 408 (2014)
6. J. Romero, J. Charry, H. Nakai, A. Reyes, *"Improving quasiparticle second order electron propagator calculations with the spin-component-scaled technique*, Chem. Phys. Lett., **591** 82 (2014)
7. R. Fernandez-Maestre, A. Reyes, H.H. Hill, *"Explaining the Drift Behavior of Caffeine and Glucosamine After Addition of Ethyl Lactate in the Buffer Gas of an Ion Mobility Spectrometer*, Bull. Korean Chem. Soc., **35** 1023 (2014)
8. R. Flores-Moreno, E. F. Posada, F. Moncada, J. Romero, J. Charry, M. A. Díaz-Tinoco, S. A. González, N. F. Aguirre, A. Reyes, *LOWDIN: The Any Particle Molecular Orbital Code*, Int. J. Quant. Chem., **114** 50 (2014)
9. S. Pan, S. Jalife, J. Romero, A. Reyes, G. Merino, and P. K. Chattaraj. *Attractive Xe-Li interaction in li-decorated clusters*, Comp. Theor. Chem., **1021** 62 (2013)
10. A. Reyes, P. A. Cuervo, F. Orozco, R. Abonia, M. Duque-Norena, P. Perez, E. Chamorro, *Theoretical investigation of the selectivity in intramolecular cyclizations of some 2'-aminochalcones to dihydroquinolin-8-ones and indolin-3-ones*, J. Mol. Mod., **19** 3611 (2013)
11. M. Díaz-Tinoco, J. Romero, J. V. Ortiz, A. Reyes, R. Flores-Moreno. *A generalized any particle propagator theory: prediction of proton affinities and acidity properties with the proton propagator*, J. Chem. Phys., **138** 194108 (2013)
12. N. F. Aguirre, E.F. Posada, P. Villareal, G. Delgado-Barrio, M. Biczysko, A. Mitrushchenkov, A. Reyes, M.P. de Lara-Castells, *Including nuclear quantum effects into highly correlated electronic structure calculations*, J. Chem. Phys., **138** 184113 (2013)

13. F. S. Moncada, S. D. Cruz, A. Reyes, *Electronic properties of atoms and molecules containing one and two negative muons*, Chem. Phys. Lett., **570** 16 (2013)
14. F. Moncada, L. Uribe. J. Romero, A. Reyes, *Hydrogen Isotope Effects on Covalent and Non-covalent Interactions: the Case of Protonated Rare Gas Clusters*, Int. J. Quant. Chem., **113** 1556 (2013)
15. K. Pineda-Urbina, R. D. Guerrero, A. Reyes, Z. Gomez-Sandoval, R. Flores-Moreno, *Shape entropy's response to molecular ionization*, J. Mol. Mod., **19** 1677 (2013)
16. J. González, E. Florez, J. Romero, A. Reyes, A. Restrepo, *Microsolvation of Mg^{2+} , Ca^{2+} : strong influence of formal charges in hydrogen bonding networks*, J. Mol. Mod., **19** 1763 (2013)
17. S. Pan, M. Contreras, J. Romero, A. Reyes, G. Merino, P. K. Chattaraj, *C₅Li₇⁺ and O₂Li₅⁺ as Noble Gas Trapping Agents*, Chem. Eur. J., **19**, 2322 (2013)
18. N. Nuñez, A. Reyes, R. Quevedo, *Hydrogen bond assisted synthesis of azacyclophanes from L-tyrosine derivatives*, Tetrahedron Lett., **53** 530 (2012)
19. F. Moncada, R. Flores, A. Reyes, *Non-Born-Oppenheimer density functional theory calculations with cubic scaling*, Chem. Phys., **400** 103 (2012)
20. F. Moncada, D. Cruz, A. Reyes, *Muonic alchemy: Transmuting elements with the inclusion of negative muons*, Chem. Phys. Lett., **539-540** 209 (2012)
21. J. Romero, E. Posada, R. Flores-Moreno, A. Reyes, *A generalized any particle propagator theory: Assessment of nuclear quantum effects on electron propagator calculations*, J. Chem. Phys., **137** 074105 (2012)
22. D. V. Moreno, S. A. González, A. Reyes, *Turning symmetric an asymmetric hydrogen bond with the inclusion of nuclear quantum effects*, J. Chem. Phys., **134** 024115 (2011)
23. E. F. Posada, F. Moncada, A. Reyes, *Optimización del paquete computacional para el cálculo de estructura núcleo-electrónica APMO*, Rev. Colomb. Quim., **40** 35 (2011)
24. J. Romero, A. Reyes, J. David, A. Restrepo, *Understanding microsolvation of Li⁺: Structural and energetical analyses*, Phys. Chem. Chem. Phys., **13** 15624 (2011)
25. R. Quevedo, I. Ortiz and A. Reyes, *Synthesis and conformational analysis of Azacyclophanes from L-Tyrosine*, Tetrahedron Lett., **51** 1216 (2010)
26. S. A. González, A. Reyes, *Hydrogen isotope effects on the He₂H⁺ complex using the APMO-MP2 method*, Int. J. Quant. Chem., **110** 689 (2010)
27. F. Moncada, S. A. González, A. Reyes, *First principles investigation of hydrogen isotope effects in (XSO₄-H-SO₄X)⁻ (X = H, K) complexes*, Mol. Phys., **108** 1545 (2010)
28. D. V. Moreno, S. A. González and A. Reyes, *Secondary hydrogen isotope effects on the structure and stability of cation-π complexes (Cation = Li⁺, Na⁺, K⁺ and π = Acetylene, Ethylene, Benzene)*, J. Phys. Chem. A, **114** 9231 (2010)
29. J. Romero, A. Reyes and J. Wist, *Secondary deuterium isotope effects on the acidity of glycine*, Spectrochim. Acta. Part A, **77** 845 (2010)

30. A. Rivera, D. Moyano, M. Maldonado, J. Ríos-Motta, A. Reyes, *FTIR and DFT studies of the proton affinity of small aminal cages*, Spectrochim. Acta, Part A, **74** 588 (2009)
31. S. A. González, A. Reyes, *Implementación del método del gradiente analítico de la energía en al teoría del orbital molecular nuclear y electrónico*, Rev. Colom. Quim., **38** 109 (2009)
32. N. Forero, S. A. González, A. Reyes, *Estudio teórico del efecto isotópico de hidrógeno en el aducto borano-carbonilo*, Rev. Colom. Quim., **38** 135 (2009)
33. I. Ortiz, S. A. González, A. Reyes, *Estudio del efecto de isótopo de hidrógeno en los complejos MH ··· HF (M: Li, Na)*, Rev. Colom. Quim., **38** 143 (2009)
34. S. A. González, N. F. Aguirre, A. Reyes, *APMO: A computer program based on the electronic and non-electronic molecular orbital theory for studies of nuclear quantum effects*, Rev. Colomb. Quim., **37** 93 (2008)
35. S. A. González, N. F. Aguirre, A. Reyes, *Theoretical investigation of isotope effects: The Any-Particle Molecular Orbital code*, Int. J. Quant. Chem., **108** 1742 (2008)
36. G. A. Parada, D. Fernández, A. Reyes, M. F. Suárez and L. Fadini, *Síntesis y estudio teórico DFT de compuestos de Ru(II) con ligantes ferrocenílicos para aplicaciones electroquímicas*, Rev. Colomb. Quim., **36** 186 (2007)
37. A. B. Pacheco, B. Thorndyke, A. Reyes, and D. A. Micha, *Quantum dynamics of an excited alkali atom in a noble gas cluster: Lithium Attached to a Helium Cluster*, J. Chem. Phys., **127** 244504 (2007)
38. A. B. Pacheco, A. Reyes, D. A. Micha, *First principles dynamics of light emission in alkali atom-noble gas atom collisions at 10keV*, J. Chem. Phys., **125** 154313 (2006)
39. A. B. Pacheco, A. Reyes, D. A. Micha, *First principles dynamics of light emission and absorption during alkali atom - noble gas atom interactions*, Phys. Rev. A, **74** 062714 (2006)
40. A. Reyes, M. V. Pak, and S. Hammes-Schiffer, *Investigation of isotope effects with the nuclear-electronic orbital method*, J. Chem. Phys., **123** 014303 (2005)
41. A. Reyes, and D. A. Micha, *Dynamics of electronic excitation in collisions of alkali atoms with noble-gas atoms using atomic core potentials*, J. Chem. Phys., **119** 12308 (2003)
42. A. Reyes, and D. A. Micha , *Dynamics of spin-orbit recoupling in collisions of alkali atoms with noble-gas atoms using atomic core potentials*, J. Chem. Phys., **119** 12316 (2003)
43. A. Reyes, D. A. Micha, and K. Runge, *First principles dynamics of Li+He collisional excitation using atomic core potentials*, Chem. Phys. Lett., **363** 441 (2002)