

## Curriculum Vitae Andrés Reyes

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### I EDUCATION

1997 BSc 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, Bogota, Colombia  
2013-2014 Visiting Professor, Institute of Physics, University of São Paulo, São Paulo, Brazil  
2013-present Professor of Chemistry, Universidad Nacional de Colombia, Bogota, Colombia

### III PUBLICATION

#### III.1 Submitted

1. R. D. Guerrero, C. A. Arango, A. Reyes, *Experimentally Attainable Optimal Pulse Shapes Obtained with the Aid of Genetic Algorithms*, J. Chem. Phys, Submitted (2015)

#### III.2 Published

1. E. Posada, F. Moncada, A. Reyes, *Negative Muon Chemistry: The Quantum Muon Effect and the Finite Nuclear Mass Effect*, J. Phys. Chem. A, **118**, 9491 (2014)
2. J. Romero, J. Charry, R. Flores-Moreno, M. Varela, A. Reyes, *Calculation of positron binding energies using the generalized any particle propagator theory*, J. Chem. Phys., **141**, 114103 (2014)
3. J. Charry, J. Romero, M. Varela, A. Reyes, *Positron binding energies of amino acids with the generalized any-particle propagator method*, Phys. Rev. A, **89** 052709 (2014)
4. 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)
5. H. J. Bohórquez, A. Reyes, *The atomic Pauli energy grows exponentially with the electronic localization*, Mol. Phys., **112** 416 (2014)

6. 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)
7. 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)
8. 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)
9. 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)
10. 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)
11. 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)
12. 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)
13. 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)
14. 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)
15. 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)
16. 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)
17. 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)
18. J. González, E. Florez, J. Romero, A. Reyes, A. Restrepo, *Microsolvation of Mg<sup>2+</sup>, Ca<sup>2+</sup>: strong influence of formal charges in hydrogen bonding networks*, J. Mol. Mod., **19** 1763 (2013)
19. 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)
20. N. Nuñez, A. Reyes, R. Quevedo, *Hydrogen bond assisted synthesis of azacyclophanes from L-tyrosine derivatives*, Tetrahedron Lett., **53** 530 (2012)

21. F. Moncada, R. Flores, A. Reyes, *Non-Born-Oppenheimer density functional theory calculations with cubic scaling*, Chem. Phys., **400** 103 (2012)
22. F. Moncada, D. Cruz, A. Reyes, *Muonic alchemy: Transmuting elements with the inclusion of negative muons*, Chem. Phys. Lett., **539-540** 209 (2012)
23. 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)
24. 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)
25. 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)
26. J. Romero, A. Reyes, J. David, A. Restrepo, *Understanding microsolvation of Li<sup>+</sup>: Structural and energetical analyses*, Phys. Chem. Chem. Phys., **13** 15624 (2011)
27. R. Quevedo, I. Ortiz and A. Reyes, *Synthesis and conformational analysis of Azacyclophanes from L-Tyrosine*, Tetrahedron Lett., **51** 1216 (2010)
28. S. A. González, A. Reyes, *Hydrogen isotope effects on the He<sub>2</sub>H<sup>+</sup> complex using the APMO-MP2 method*, Int. J. Quant. Chem., **110** 689 (2010)
29. F. Moncada, S. A. González, A. Reyes, *First principles investigation of hydrogen isotope effects in (XSO<sub>4</sub>-H-SO<sub>4</sub>X)<sup>-</sup> (X = H, K) complexes*, Mol. Phys., **108** 1545 (2010)
30. D. V. Moreno, S. A. González and A. Reyes, *Secondary hydrogen isotope effects on the structure and stability of cation- $\pi$  complexes (Cation = Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup> and  $\pi$  = Acetylene, Ethylene, Benzene)*, J. Phys. Chem. A, **114** 9231 (2010)
31. J. Romero, A. Reyes and J. Wist, *Secondary deuterium isotope effects on the acidity of glycine*, Spectrochim. Acta. Part A, **77** 845 (2010)
32. A. Rivera, D. Moyano, M. Maldonado, J. Ríos-Motta, A. Reyes, *FTIR and DFT studies of the proton affinity of small aminated cages*, Spectrochim. Acta, Part A, **74** 588 (2009)
33. S. A. González, A. Reyes, *Implementación del método del gradiente analítico de la energía en la teoría del orbital molecular nuclear y electrónico*, Rev. Colomb. Quim., **38** 109 (2009)
34. N. Forero, S. A. González, A. Reyes, *Estudio teórico del efecto isotópico de hidrógeno en el aducto borano-carbonilo*, Rev. Colomb. Quim., **38** 135 (2009)
35. I. Ortiz, S. A. González, A. Reyes, *Estudio del efecto de isótopo de hidrógeno en los complejos MH  $\cdots$  HF (M: Li, Na)*, Rev. Colomb. Quim., **38** 143 (2009)
36. 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)
37. 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)

38. 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 ferrocénicos para aplicaciones electroquímicas*, Rev. Colomb. Quim., **36** 186 (2007)
39. 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)
40. 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)
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43. 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)
44. 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)
45. 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)