J. Ulises Reveles

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Education

Ph.D. – Chemical Sciences	Center of Research and Advanced Studies, Mexico, Advisor: Prof. Dr. Andreas M. Köster,	2004
PhD Thesis Title:	"Geometry Optimization in LCGTO-DFT Methods with Auxiliary Functions".	
B.Sc. – Chemical Engineering	National University of Mexico (UNAM), Mexico.	2000

Professional Experience

Visiting Research Associate Professor	University of Texas el Paso, TX	May/2013 - Present
Assistant Professor	Virginia Commonwealth Univ., Richmond, VA	Aug/2014 - Present
Instructor/Researcher	Virginia Commonwealth Univ., Richmond, VA	Aug/2010 – Jul/2014
Certified MCAT Physics and GChem Instructor	The Princeton Review Co., Richmond, VA	Feb/2012 - Present
Research Assistant Professor	Virginia Commonwealth Univ., Richmond, VA	Aug/2009 - Jul/2010
Postdoctoral Associate	Virginia Commonwealth Univ., Richmond, VA	Jan/2005 - Jul/2009
Postdoctoral Associate	Center of Research and Advanced Studies, Mexico City, Mexico	Sep.-Dec. 2004
Research and Development Assistant	Beisa/ Schering Plough México City	Jul.-Dec. 1998

Research and Teaching Projects

- **J.U. Reveles, *"Implementing Delocalized Internal Coordinates in the Naval Research Laboratory Molecular Orbital Library (NRLMOL) code** and building a framework for future collaborations with University of Texas el Paso (UTEP)"* (May. – Aug. 2013).
- **J.U. Reveles**, "***Development of Process Oriented Guided Sessions for Physics"* (Feb. – Jul. 2012).**
  Physics Department @ VCU / $5,000.Advised a group of 10 undergrads and one Masters student.
  The new developed sessions are now used by ~500 VCU students every semester.

- Anita Nadal, **J.U. Reveles**, Lynn Pelco, ***"VERDE: Efficient use of energy resources in Europe and the benefit of alternative energy sources in immigrant communities".*** GEO International Initiative Strategic Award Program @ VCU/ $20,000.
- E. Howard and **J.U. Reveles, *"Crossing the River: Bridging the Education Gap – Enhancing the First Spanish GED preparation program in Richmond".*** Council of Community Engagement Grant @ VCU (2013-2014) $17,500.
- A.Y. Leon and **J.U. Reveles, *"Crossing the River: Bridging the Education Gap – Enhancing the First Spanish GED preparation program in Richmond".*** Council of Community Engagement Grant @ VCU (2013-2014). Selected as finalist and received partial funding.

Work Status: Authorized to work in the US for any employer (Green card status since Jan/2010 -NIW EB-2 program).

Languages: English (fluent) and Spanish (mother tongue).

Teaching Experience

Virginia Commonwealth University
Aug. 2009 - Current

- **Taught 55** Chemistry, Physics, Science, and General Education undergraduate courses: Introductory Chemistry, General Chemistry, General Physics I & II, Calculus-based Physics I & II (Recitations), Modern Physics Laboratory, Sci. Techno, & Soc. (Honors), and Energy!.
- Received average rating of 3.91 (Instructor), in a scale from 1-5, by students' evaluations.
- Course size ranged from 6 to 430 students.

The Princeton Review Company
Feb. 2012 – Current

- Taught 3 MCAT Physics courses.
- Taught 1 MCAT General Chemistry course.
- Course size ranged from 6 to 20 students.

Sacred Heart Catholic Church, Richmond, VA
Sep. - Dec. 2011, Sep.2012-

- Volunteer Instructor of GED course.
- Course size ranged from 4 to 20 students.

Academic Honors and Awards

- 2013 Service Learning Award @ VCU / $1,000
- 2013 GEO International Initiative Strategic Award Program @ VCU / $20,000.
- PI of Research project to develop Process Oriented Guided sessions (Feb – May 2012). Supported by the Physics Department @ VCU / $5000.00.

- National Researcher Level I by SNI (Mexico's Scientific Research Bureau), 2008 -10.
- National Researcher Level II by SNI, 2013 -16.

Research Experience

- Cluster reactivity in studies of CO oxidation by transition metal oxides with potential catalytic applications.
- Electronic structure studies of magnetic nanoparticles, cluster and cluster assemblies.
- Discovery of multiple valence and magnetic cluster superatoms.
- Structure activity relations of organic compounds.
- Organic Chemistry Synthesis and characterization of new chiral compounds.
- Analytical skills, experience in scientific programming and development of new algorithms for the efficient ab-initio calculation of large molecular systems.
- Development of algorithms for local and global geometry optimization.
- Coauthor/developer of the deMon2k (density of Montreal) computational software package.

Professional Activities

- Faculty Advisor for the Society of Physics Students (SOPS) @ VCU.
- Member of search committee for two new positions in the Chemistry Department @ VCU: Physical Chemistry and Analytical Chemistry.
- Member of PhD committee for the Doctorate Program: Mechanical and Nuclear Eng. Dpt. @ VCU.
- Editor of the 2012 MRS proceedings.
- Co-Organizer of Symposium "**Advances in Computational Materials Science",** International Materials Research Congress (IMRC) 2011-2014, Cancun Mexico.
- Local organizer for the 5th International Conference on Theory of Atomic and Molecular Clusters (**TAMC**), Richmond, VA.USA, June 2006.
- Reviewer of Grant Proposals for the Mexico's Scientific Research Bureau.
- Reviewer of Grant Proposals for the Chile's National Scientific and Technological Bureau.
- Referee for the Journals
  - Journal of Molecular Catalysis A: Chemical
  - Chemical Physics Letters
  - Phys. Chem. Chem. Phys.
  - Advances in Science and Engineering (Avances en Ciencias e Ingenieria)
  - Journal of Molecular Modeling
  - Journal of Physical Chemistry
  - Journal of Chemical Physics

Scientific Publications

Book Chapters

Reveles, J.U., Chemistry in the computer: We can see the molecules, In ***Science and Technology from Cinvestav***; Parra, A.F., Ed.; Cinvestav, Mexico: **2006**, 156-172.

Köster, A.M.; Calaminici, P.; Gomez, Z.; **Reveles, J.U.**, Density Functional Theory Calculation of Transition Metal Clusters, In ***Reviews in Modern Quantum Chemistry (A Celebration of the***

contributions of Robert G. Parr); Sen, K.D., Ed.; World Scientific, Singapore: **2002**, 1439-1475.

Peer-Reviewed Publications

Papers in Preparation

57) **Reveles, J.U** "Ionic solid based on Superatom Clusters"
J. Chem. Phys.. To be submitted on Aug. 2014.

Accepted Papers

2014

56) Zamora, A.Y.; **Reveles, J.U.;** Mejia-Olvera, R.; Baruah, T.; Zope, R.R. "CO oxidation on MgO deposited clusters" "FeO_2/MgO(100) Supported Cluster: Computational Pursual for a Low-Cost CO and Low-Temperature Nanocatalyst"
Chem. Phys. Lett. Accepted on July 2014.

Published Papers

2013

55) González-Ramírez, H.; **Reveles, J.U.**; Gomez-Sandoval, Z. "High Magnetic Moments on Binary Ytrium-Alkali Superatoms",
Chem. Phys. Lett. 583, 97-102 (2013).

54) Medel, V.M.; **Reveles, J.U.**; Khanna, S.N. "Robust Magnetic Moments on Impurities in Metallic Clusters: Localized Magnetic States in Superatoms",
Submitted to ***J. Phys. Chem. A*** 117(20), 4297–4303 (2013).

53) Xinxing, Z.; Yi, W.; Haopeng, W.; Alane, L.; Gerd, G.; Kit, H.B.; **Reveles, J.U.**; Khanna, S.N. "On the Existence of Designer Magnetic SuperatomsMagnetism of Electrons in Superatoms",
J. Am. Chem. Soc. 135, 4856−4861 (2013).
Spotlights on: Recent JACS Publications J. Am. Chem. Soc. 2013, 135, 4575−457, Chemical & Engineering News and more than other 100 websites worldwide.

2012

52) Luo, Zhixun; Gamboa, G.; Smith, J.; Reber, A.C.; **Reveles, J.U.**; Khanna, S.N.; Castleman, A. W., Jr. "Spin Accommodation and Reactivity of Silver Clusters with Oxygen: The Enhanced Stability of Ag_{13}^-".
J. Am. Chem. Soc. **134**, 18973 (2012).

51) Medel, V.M.; **Reveles, J.U.**; Khanna, S.N. "Magnetism of Electrons in Superatoms",
J. Appl. Phys. **112**, 064313 (2012).

50) Medel, V.M.; Reber, A.C.; **Reveles, J.U.**; Khanna, S.N. "Metallic and Molecular Orbital Concepts in XMg_8 clusters, X=Be-F", ***J. Chem. Phys.*** **136**, 134311 (2012).

49) **Reveles, J.U.**; Koster, A.M.; Calaminici, P.; Khanna, S.N. "Pd_{13} Structural Changes upon charge and Oxidation/Reduction", ***J. Chem. Phys.*** **136**, 114505 (2012).

48) Chauhan, V.; Medel, V.M.; **Reveles, J.U**.; Khanna, S.N.; Sen. P. "Shell Magnetism in transition Doped Calcium Superatom", ***Chem. Phys. Lett.,*** **528**, 39 (2012).

47) Quintanar C.; Caballero R.; **Reveles J.U.**; Khanna, S.N. " Nature of the bonding, surface relaxation and charge transfer of Au dimers on an MgO(100) surface", ***Rev. Mex. Fis.*** **58**, 77-85 (2012).

46) Geudtner, G.; Koster, A.M.; Calaminici, P.; Goursot, A.; Dominguez-Soria, V.D.; Gamboa-

Martinez, G.U.; Vasquez-Perez, J.M.; **Reveles, J.U.**; Vela, A.; Salahub, D.R. "deMon2k", ***WIREs Computational Molecular Science,*** **2**(4), 548-555 (2012).

2011

45) Köster, A.M.; Calaminici, P.; Orgaz, E.; Roy, D.R.; **Reveles, J.U**.; Khanna, S.N. "On the Pd13 ground state", ***J. Am. Chem. Soc.,*** **133**, 12192 (2011).

44) Medel, V.M.; **Reveles, J.U**.; Reber, A.C.; Khanna, S.N.; Castleman A.W. Jr. "Closed-shell to Split-shell Stability of Iso-valent Clusters", ***Phys. Rev. B,*** **84**, 075435 (2011).

43) Medel, V.M.; **Reveles, J.U**.; Khanna, S. N.; Chauhan, V.,; Sen, P. "Hund's Rule in Transition Metal Doped Clulsters", ***Proc. Natl. Acad. Sci. USA,*** **108**, 10062 (2011). ***Featured on the Physorg., Sciencedaily, and more than other 50 websites worldwide.***

42) Carrol, K.; **Reveles, J.U**.; Shultz, M.D.; Khanna, S. N.; Carpenter, E. E. "Preparation of elemental Cu and Ni nanoparticles by the polyol method: An experimental and theoretical approach", ***J. Phys. Chem. C,*** **6**, 2656 (2011).

2010

41) Melko, J.J.; Ong, S.V.; Gupta, U.; **Reveles, J.U.**; D'Emidio, J.; Khanna, S.N.; Castleman, A.W. Jr., "Anion Photoelectron Spectroscopy and First-Principles Study of Pb_xIn_y Clusters", ***J. Phys. Chem. C,*** **114**, 2097 (2010)

40) Melko, J.J.; Ong, S.V.; Gupta, U.; **Reveles, J.U.**; D'Emidio, J.; Khanna, S.N.; Castleman, A.W. Jr., "Resilient Aromaticity in Lead-Indium Clusters", ***Chem. Phys. Lett.*** **500**, 196 (2010).

39) Sobhy, M.A., Casalenuovo, K.; **Reveles, J.U.**; Gupta, U.; Khanna, S.N.; Castleman, A.W. Jr., "Photoelectron imaging and density-functional investigation of Bismuth and Lead anions solvated in ammonia clusters", ***J. Phys. Chem. A***, **114**, 11353 (2010).

38) Gupta, U.; **Reveles, J.U.**; Melko, J.J.; Khanna, S.N.; Castleman; A.W., Jr., "Origins of Stability in Mixed Bismuth-Indium Clusters", ***J. Phys. Chem. C***, **114**, 15963 (2010).

37) **Reveles, J.U.**; Koster, A.M.; Khanna, S.N.; Quintanar, C., "Surface Oxygen Diffusion into Neutral, Cationic, and Dicationic Oxygen Vacancies on MgO(100) Surfaces", ***J. Phys. Chem. C***, **114**, 12265 (2010).

36) **Reveles, J.U.**; Sen, P.; Pradhan, K., Roy, D.R.; Khanna, S.N., "Effect of Electronic and Geometric Shell Closures on the Stability of Neutral and Anionic $TiNa_n$ (n=1-13) clusters", ***J. Phys. Chem. C,*** **114**, 10739 (2010).

35) Pradhan, K.; **Reveles, J.U.**; Sen, P.; Khanna, S.N., "Enhanced Magnetic Moments of Alkali Metal Coated Sc Clusters: New Magnetic Superatoms", ***J. Chem. Phys.***, **132**, 124302 (2010).

34) **Reveles, J.U**.; Johnson, G.E.; Khanna, S.N.; Castleman, Jr., A.W., "Reactivity Trends in the Oxidation of CO by Anionic Transition Metal Oxide Clusters", ***J. Phys. Chem. C***, **114**, 5438, 2010.

33) Melko, J.; Clayborne, P.; Jones, C.; **Reveles, J.U.**; Gupta, U.; Khanna, S.N.; Castleman, Jr., A.W., "A Combined Experimental and Theoretical Study of Al_nX (n = 1-6, X = As, Sb) Clusters: Evidence of Aromaticity and the Jellium Model", ***J. Phys. Chem. A***, **114**, 2045 (2010).

2009

32) He, H.; Pandey, P.; **Reveles, J.U.**; Khanna, S.N.; Karna, S.P., "Highly Efficient (Cs_8V) Superatom-based Spin-polarizer", ***Appl. Phys. Lett.***, **95**, 192104 (2009).

31) Gupta, U.; **Reveles, J.U**.; Melko, J.J.; Khanna, S.N.; Castleman, Jr., A.W., "Electron Delocalization in a Non-Cyclic All-Metal III-V Cluster", ***Chem. Phys. Lett.***, **2009**, 480, 189.

30) **Reveles**, **J.U**.; Clayborne, P.A.; Reber, A.C.; Khanna, S.N.; Pradhan, K.; Sen, P.; Pederson, M.R., "Designer Magnetic Superatoms", ***Nat. Chem.***, **2009**, 1, 310. ***Research Highlights papers in Nature Chemistry 2009, 1, 260, and New Scientist June 2009. Featured on the Physorg., Sciencedaily, and more than other 200 websites worldwide.***

29) M.A. Sobhy, M. A.; **Reveles, J.U.**; Gupta, U.; Khanna, S.N.; Castleman, Jr. A.W., "Photoelectron Imaging and Theoretical Investigation of Bimetalic $Bi_{1-2}Ga_{0-2}^-$ and lead Pb_{1-4}^- cluster anions", ***J. Chem. Phys.*** **2009**, 130, 054304.

28) Gupta, U.; **Reveles, J.U.**; Melko, J.J.; Khanna, S.N.; Castleman, Jr. A.W., "Electronic Structure of $Bi_3Ga_y^-$ Semiconductor Cluster and the Special Stability of $Bi_3Ga_2^-$ - A Gas Phase Zintl Analog", ***Chem. Phys. Lett.*** **2009**, 4, 223.

2008

27) Jones Jr. C.; Clayborne, P.; **Reveles, J.U.**; Melko, J.J.; Gupta, U.; Khanna, S.N.; Castleman, Jr., A.W., "Al_nBi Clusters: Transitions Between Aromatic and Jellium Stability", ***J. Phys. Chem. A,*** **2008**, 112, 13316.

26) Johnson, G.E.; **Reveles, J.U.**; Reilly, N.M.; Tyo, E.C.; Khanna, S.N.; Castleman, Jr., A.W., "Influence of Stoichiometry and Charge State on the Structure and Reactivity of Cobalt Oxide Clusters with CO", ***J. Phys. Chem. A,*** **2008**, 112, 11330

25) Caballero, R.; Quintanar, C.; Köster, A.M.; Khanna, S.N.; **Reveles, J.U.**, "Structural and Electronic Properties of Au and Au_2 on an MgO(100) Surface: A DFT Cluster Embedding Approach", ***J. Phys. Chem. A,*** **2008**, 112, 11330

24) Pradhan, K.; Sen, P.; **Reveles, J.U**.; Khanna, S.N., "First-principles stuy of $TMNa_n$ (TM = Cr, Mn, Fe, Co, Ni; n = 4-7) Clusters", ***J. Phys.: Condens. Matter*** **2008**, 20, 255243.

23) Pradhan, K.; Sen, P.; **Reveles, J.U**.; Khanna, S.N., "Enhanced Magnetic Moments on $TMNa_4$ clusters: (TM = Sc, Ti, V; n = 4, 5, 6)", ***Phys. Rev. B.*** **2008**, 77, 045408.

2007

22) Clayborne, P.; Jones, N.O.; Reber, A.C.; **Reveles, J.U**.; Qian, M.C.; Khanna, S.N., "Superatoms and their assemblies based on Alkali and Super-alkali Motifs", ***J. Comp. Meth. Sci. Eng. 2007***, 7, 417.

21) Knappenberger, Jr., K.L.; Clayborne, P.A.; **Reveles, J.U.**; Sobhy, M.A.; Jones, Jr., C.E.; Gupta, U.U; Khanna, S.N.; Iordanov, I.; Sofo, J.; Castleman, Jr.. A.W., "Anion Photoelectron spectroscopy and Density Functional Investigation of Diniobium Carbon Clusters", ***ACS Nano*** **2007**, 4, 319.

20) **Reveles, J.U**.; Calaminici, P.; Beltrán, M.R.; Köster, A.M.; Khanna, S.N., "H_2O Nucleation around Au^+", ***J. Am. Chem. Soc.*** **2007**, 129, 15565. ***Research Highlights paper in Nature Physics 4, 9 (2008).***

19) Reilly, N.M.; **Reveles, J.U**.; Johnson, G.E.; M.del Campo, J.; Khanna, S.N.; Köster, A.M.; Castleman, Jr., A.W. "Experimental and Theoretical Study of the Structure and Reactivity of $Fe_{1-2}O_{1-5}^+$ with CO", ***J. Phys. Chem. C,*** **2007**, 111, 19086.

18) Reilly, N.M.; **Reveles, J.U**.; Johnson, G.E.; Khanna, S.N.; Castleman, Jr., A.W., "Experimental and Theoretical Study of the Structure and Reactivity of $Fe_{1-2}O_{1-6}^-$ Clusters with CO",

J. Phys. Chem. A, 2007, 111, 4158.

17) Kimble, M.L.; Castleman, Jr., A.W.; **Reveles, J.U**.; Khanna, S.N., "On the Magic Character of Al_6Au", ***Collect. Czech. Chem. Commun.*** **2007**, 72, 185.

16) Shultz, M.D.; **Reveles, J.U**.; Khanna, S. N.; Carpenter, E. E. "Reactive Nature of Dopamine as a Surface Functionalization Agent in Iron Oxide Nanoparticles", ***J. Am. Chem. Soc.*** **2007,** 129, 2482.

15) Reilly, N.M.; **Reveles, J.U**.; Johnson, G.E.; Khanna, S.N.; Castleman, Jr., A.W., "Influence of Charge State on the Reaction of $FeO_3^{+/-}$ with Carbon Monoxide", ***Chem. Phys. Lett.*** **2007**, 435, 295.

2006

14) **Reveles, J.U**.; Khanna, S.N.; Roach, P.J.; Castleman, Jr., A.W., "Multiple Valence Superatoms", ***Proc. Natl. Acad. Sci.*** **2006**, 103, 18405. ***Research Highlights papers in C&EN News 2006, Nov. 21, and Nature Materials 2006, Nov. 23.***

13) Jardillier, N.; Berthomieu, D.; Goursot, A.; **Reveles, J.U**.; Köster, A.M., "Theoretical Study of $Cu^{I}Y$ Zeolite: Structure and Electronic Properties", *J. Phys. Chem. B* **2006**, 110, 18440.

12) **Reveles, J.U**.; Khanna, S.N., "Electronic counting rules for the stability of metal-silicon clusters", ***Phys. Rev. B*** **2006**, 74, 035435.

11) Reber, A.C.; Clayborne, P.A.; **Reveles, J.U.;** Khanna, S.N.; Castleman, Jr., A.W.; Ali. A., "Silicon oxide nanoparticles reveal the origin of silicate grains in circumstellar environments", ***Nano Letters*** **2006**, 6, 1190. ***Research Highlights papers in New Scientist July 2006. Featured on the NASA website.***

10) **Reveles, J.U**.; Khanna, S.N.; Köster, A.M., "Equivalent delocalized internal coordinates", ***J. Mol. Struct. THEOCHEM*** **2006**, 762, 171.

9) King-Diaz, B.; Macias-Ruvalcaba, N.A.; Aguilar-Martiez, M.; Calaminici, P.; Köster, A.M.; Gomez-Sandoval, Z.; **Reveles, J.U**.; Lotina-Hennsen, B.,"2-[(R-Phenyl)amine]-1,4-naphthalendiones as Photosystem I Electron Acceptors. Structure-activity Relationship of m- and p-PAN Compounds with QSAR analysis", ***J. Photochem. Photobiol. B: Biology*** **2006,** 83, 105.

8) Jones, N.O.; **Reveles, J.U**.; Khanna, S.N.; Bergeron, D.E.; Roach, P.J.; Castleman, Jr. A.W. "Structural, electronic, and chemical properties of multiply iodized aluminum clusters", ***J. Chem. Phys.*** **2006**, 124, 154311.

2005

7) Bergeron, D.E.; Roach, P.J.; Castleman, Jr., A.W.; Jones, N.O.; **Reveles, J.U**.; Khanna, S.N., "Reactions of $Al_nI_x^-$ with methyl iodide: The enhanced stability of Al_7I and the chemical significance of active centers", ***J. Am. Chem. Soc.*** **2005**, 127, 16048.

6) **Reveles, J.U.;** Khanna, S.N., "Nearly Free Electron Gas in a Silicon Cage", ***Phys. Rev. B.*** **2005**, 72, 165413.

5) **Reveles, J.U.;** Heine, T.; Köster, A.M., "^{13}C NMR pattern of $SC_3N@C_{68}$. Structural assignment of the first fullerene with adjacent pentagons", ***J. Phys. Chem. A*** **2005**, 109, 7068.

4) Merino, G.; **Reveles, J.U**.; Mendez-Rojas, M.A.; Escalante, S., "What is it, What is for and How to Build a Z-Matrix", ***Educacion Quimica*** **2005**, 16, 88.

2004

3) Köster, A.M.; **Reveles, J.U**.; M. del Campo, J., "Calculation of exchange-correlation potentials with auxiliary function densities", ***J. Chem. Phys.*** **2004**, 121, 3417.

2) Köster, A.M.; Flores-Moreno, R.; **Reveles, J.U**., "Efficient and Reliable Numerical Integration of Exchange-Correlation Energies and Potentials", ***J. Chem. Phys.*** **2004**, 121, 681.

1) **Reveles, J.U.**; Köster, A.M. "Geometry optimization in density functional methods**",** ***J. Comput. Chem.*** **2004,** 25, 1109.

Invited Talks

- *Structural Oscillations of Pd_{13} Upon Charge and Oxidation-Reduction*
  XXI International Materials Research Congress,
  Cancun, Mexico, Aug. 2012.
- *Nanoclusters: Designing New Stable Clusters and Catalysts.*
  Theoretical Chemistry for the XXI Century, UNAM,
  Mexico City, Mexico. September 2011.
- *Nanoclusters: Extending the Periodic Table and Designing New Catalysts.*
  Inorganic Chemistry Conference 2011,
  Guadalajara, Mexico, June 2011.
- *Experimental and Theoretical Investigation of Oxidation of CO by Transition Metal Oxide Clusters.*
  The 6th International Conference on Theory of Atomic and Molecular Cluster (TAMC),
  Mexico City, Mexico. June 2010.
- *Superatoms: Building new Materials.*
  8th Workshop of Chemistry Cinvestav, Center for Research and Advanced Studies,
  Mexico City, Mexico. Nov. 2008.
- *Nearly Free Electron Gas in a Silicon Cage.*
  XIV International Materials Research Congress,
  Cancun, Mexico, Aug. 2005.

Contributed Presentations

- March Meeting 2012, Boston. Mass., March 2012.
- March Meeting 2011, Houston, Texas, March 2011.
- March Meeting 2010, Portland, Oregon, March 2010.
- March Meeting 2009, Pittsburgh, Pennsylvania, March 2009.
- March Meeting 2008, New Orleans, Louisiana, March 2008.
- International Symposium of Theory of Atomic and Molecular Clusters, TAMC5, Richmond, Virginia, May 2008.
- 5th Mexican Meeting of Theoretical Physical Chemistry, San Luis Potosí, Mexico, Nov. 2006.
- Center for Applied Physics and Advanced Technology, National University of Mexico (UNAM), Queretaro, Mexico, June 2006.
- March Meeting 2006, Baltimore Maryland, March 2006.
- 2nd Mexican Meeting of Theoretical Physical Chemistry, Guanajuato, Mexico, Nov. 2003

- 4th International deMon Developers Workshop, Laboratory of Theoretical Chemistry, Royal Institute of Technology, Stockholm, Sweden, April 2003.
- 1st Mexican Meeting of Theoretical Physical Chemistry, Cuernavaca, Mexico, Nov. 2002.
- 89th Pharmaceutic National Conference, Colima, Mexico, May 2002.
- 3rd International deMon Developers Workshop, Department of Physical Chemistry, University of Geneva, Geneva, Switzerland, April 2002.
- 3rd Workshop of Chemistry Cinvestav, Mexico City, Nov. 2001.
- 2nd Workshop of Chemistry Cinvestav, Mexico City, Oct. 2000.

Design and Development of Software

Coauthor of the deMon2k scientific program (around 10,000 lines of FORTRAN code) developed and used by scientific groups all over the world.
The deMon2k (density of Montréal) is a software package for density functional theory (DFT) calculations. It uses the linear combination of Gaussian-type orbital (LCGTO) approach for the self-consistent solution of the Kohn-Sham (KS) DFT equations.

Techniques of Expertise

Computational Chemistry Software

- deMon2k, Gaussian, NRLMOL, ADF, Gamess, Hyperchem.

Programming Languages

- Programming in UNIX and Linux operating systems using Fortran 77/90.

Scientific visualization and General purpose applications

- Blender, Molden, Molekel, VU, and Schakal, Origin
- Photoshop, MS Office, Latex, etc.

References

- Prof. Shiv N. Khanna, Commonwealth Professor — snkhanna@vcu.edu
  Physics Department, — (804)-828-1820
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  Chair of the Physics Department — (804)-828-1821
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  701 W Grace Street Richmond, VA. 23284

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  Virginia Commonwealth University,
  828 West Franklin Street, P.O. Box 842019, Richmond, VA. 23284.

- Prof. Ravi Pandey, — pandey@mtu.edu
  Physics Department, — (906)-487-2086
  Michigan Tech,

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- Prof. A.W. Castleman Jr., Evan Pugh Professor awc@psu.edu
  Department of Chemistry and Physics, (814)-865-7242
  The Pennsylvania State University,
  309 Chemistry Building, University Park, PA. 16802.