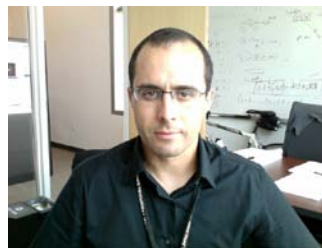


# Miguel A. Fuentes-Cabrera

Research Staff  
Center for Nanophase Materials Sciences  
Oak Ridge National Laboratory  
(865) 574-2206  
fuentescabma@ornl.gov



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## Education

University of La Laguna, Tenerife, Canary Islands, Spain  
University of La Laguna, Tenerife, Canary Islands, Spain

Physics B.A., 1993  
Physics Ph.D., 1998

## Professional Experience

2009–p Research Staff, Computer Science and Mathematics Division, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory  
2006–2009 Research Scientist I, Joint Institute for Computational Sciences, Computer Science and Mathematics Division, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory  
2002–2006 Postdoctoral Research Associate, Oak Ridge National Laboratory  
2001–2002 Postdoctoral Research Associate, North Carolina State University.  
1999–2001 Fulbright Postdoctoral Research Associate, Arizona State University.

## Honors and Awards

1999–2001 Fulbright Postdoctoral Scholar  
1994–1998 Ph. D. Fellowship, Spanish Ministry of Education

## Research Synopsis

1. *Self-Assembled Monolayers*: We use *ab initio* techniques, based on Density Functional Theory, to understand the self-assembling of molecular clusters and molecular monolayers on metallic surfaces. This work is done in collaboration with an experimental group at CNMS.
2. *Design and Synthesis of Nanomaterials*: We use classical molecular dynamics simulations to understand the de-wetting of metallic thin films and nanostructures on graphite. The goal is to control the de-wetting process so as to control the self-assembling of metallic nanoparticles. This work is done in collaboration with an experimental group at CNMS.
3. *Synthetic Biology*: *Ab-initio* techniques and classical molecular dynamics simulations are used to investigate a variety of topics within the area of Synthetic Biology, i.e. i) whether artificial DNAs could be an alternative to natural DNA for nanotechnological applications; ii) pre-biotic chemistry; iii) the use of bacterial micro-compartments for creating biofuels.

## Publications ~ 46 (Full list provided below)

### Collaborations Outside ORNL During Past Five Years

Otto F. Sankey, Arizona State University; Jerry Bernholc and Wenchang Lu, North Carolina State University; Judit E. Spöner and Jiri Spöner, Institute of Biophysics of the Czech Republic; Javier F. Luque and Modesto Orozco, Universitat de Barcelona, Spain; Rosa Di Felice, University of Modena and Reggio Emilia, Italy; Mike Baskes, Los Alamos National Laboratory; Anatoly V. Melechko, North Carolina State University; Jerzy Leszczynski, Jackson State University; Leon Petit, University of Aarhus, Denmark; Alfonso Muñoz-González, Universidad de La Laguna, Spain.

### Graduate and Postdoc Advisors

Graduate Advisor: Prof. Alfonso Muñoz-González (University of La Laguna)

Postdoc Advisors: Otto F. Sankey (Arizona State University); Celeste Sagui (North Carolina State University); Don Nicholson and Jack C. Wells (ORNL)

### Postdocs and Students Advised

- *Postdocs.*
  - Yungok Ihm, August 2011-p (co-mentored with James Morris, University of Tennessee).
  - Trung D. Nguyen, August 2011-p (co-mentored with Michael W. Brown, Oak Ridge National Laboratory).
- *Undergraduate Students.* Sponsor: Higher Education Research Experiences at Oak Ridge National Laboratory for Students.
  - Scott R. Horton, May 2009-February 2010
  - Bradley H. Rhodes, May-August 2010
  - Scott R. Horton, May-August 2011
  - Chengbo Han, May-August 2011
  - Benjamin Hulbert, August-December 2011
- *High-School Students.* Sponsor: Tennessee Governor Academy of Students
  - Shelby Vazquez, January-April 2010
  - David Calhoun, January-April 2010
  - Jacob A. Terry, November 2010-January 2011
- *Visiting Undergraduate Students from Minority Schools hosted*
  - Marquita Watkins, Jackson State University, Jackson, MS, May-July 2011.

### Publications

1. Li, Q.; Han, C.; Horton, S. R.; Fuentes-Cabrera, M.; Sumpter, B. G.; Lu, W.; Bernholc, J.; Maksymovych, P.; Pan, M.; Supramolecular Self-Assembly of  $\pi$ -Conjugated Hydrocarbons via 2D Cooperative CH/ $\pi$  Interaction, *ACS Nano*, **2011** DOI: 10.1021/nn203952e
2. Spomer, J. E.; Mladek, A.; Fuentes-Cabrera, M., Sponer, J. Fomamide-Based Prebiotic Synthesis of Nucleobases: Kinetically Accessible Reaction Route. *J. Phys. Chem. A*, **2011**, DOI: 10.1021/jp209886b
3. Sponer, J. E.; Sponer, J.; Fuentes-Cabrera, M., Prebiotic Routes to Nucleosides: A Quantum Chemical Insight into the Energetics of the Multistep Reaction Pathways. *Chem-Eur J* **2011**, *17* (3), 847-854.
4. Sponer, J. E.; Mladek, A.; Sponer, J.; Sumpter, B. G.; Fuentes-Cabrera, M., On the Geometry and Electronic Structure of the As-DNA Backbone. *J Phys Chem Lett* **2011**, *2* (5), 389-392.
5. Fuentes-Cabrera, M. R., B. H.; Baskes, M. I.; Terrones, H.; Fowlkes, J. D.; Simpson, M. L.; Rack, P. D., Controlling the Velocity of Jumping Nanodroplets Via Their Initial Shape and Temperature. *ACS Nano* **2011**, *5*(9) 7130-7136.
6. Fuentes-Cabrera, M.; Vazquez-Mayagoitia, A.; Horton, S. R.; Sumpter, B. G.; Sponer, J.; Sponer, J. E., On the Stabilization of Ribose by Silicate Minerals. *Astrobiology* **2011**, *11* (2), 115-121.
7. Fuentes-Cabrera, M.; Rhodes, B. H.; Fowlkes, J. D.; Lopez-Benzanilla, A.; Terrones, H.; Simpson, M. L.; Rack, P. D., Molecular dynamics study of the dewetting of copper on graphite and graphene: Implications for nanoscale self-assembly. *Phys Rev E* **2011**, *83* (4).
8. Fuentes-Cabrera, M.; Mladek, A.; Sponer, J.; Sumpter, B. G.; Sponer, J. E., Theoretical modeling on the kinetics of the arsenate-ester hydrolysis: implications to the stability of As-DNA. *Phys Chem Chem Phys* **2011**, *13* (23), 10869-10871.
9. Blas, J. R. H., O.; Tabares, C.; Sumpter, B. G.; Fuentes-Cabrera, M.; Orozco, M.; Ordejon, P.; Luque, F. J., Structural, Dynamical, and Electronic Transport Properties of Modified DNA Duplexes Containing Size-Expanded Nucleobases. *J. Phys. Chem. A*, **2011**.

10. Blas, J. R.; Huertas, O.; Tabares, C.; Sumpter, B. G.; Fuentes-Cabrera, M.; Orozco, M.; Ordejon, P.; Luque, F. J., Structural, Dynamical, and Electronic Transport Properties of Modified DNA Duplexes Containing Size-Expanded Nucleobases. *J Phys Chem A* **2011**, *115* (41), 11344-11354.
11. Sponer, J. E.; Vazquez-Mayagoitia, A.; Sumpter, B. G.; Leszczynski, J.; Sponer, J.; Otyepka, M.; Banas, P.; Fuentes-Cabrera, M., Theoretical Studies on the Intermolecular Interactions of Potentially Primordial Base-Pair Analogues. *Chem-Eur J* **2010**, *16* (10), 3057-3065.
12. Manjon, F. J.; Gomis, O.; Rodriguez-Hernandez, P.; Perez-Gonzalez, E.; Munoz, A.; Errandonea, D.; Ruiz-Fuertes, J.; Segura, A.; Fuentes-Cabrera, M.; Tiginyanu, I. M.; Ursaki, V. V., Nonlinear pressure dependence of the direct band gap in adamantane ordered-vacancy compounds. *Phys Rev B* **2010**, *81* (19).
13. Keffer, D. J.; Xiong, R. C.; Fuentes-Cabrera, M.; Nicholson, D. M.; Michalkova, A.; Petrova, T.; Leszczynski, J.; Odbadrakh, K.; Doss, B. L.; Lewis, J. P., Effect of Charge Distribution on RDX Adsorption in IRMOF-10. *Langmuir* **2010**, *26* (8), 5942-5950.
14. Clearfield, R.; Railsback, J. G.; Pearce, R. C.; Hensley, D. K.; Fowlkes, J. D.; Fuentes-Cabrera, M.; Simpson, M. L.; Rack, P. D.; Melechko, A. V., Reactive solid-state dewetting of Cu-Ni films on silicon. *Appl Phys Lett* **2010**, *97* (25).
15. Vazquez-Mayagoitia, A.; Huertas, O.; Brancolini, G.; Migliore, A.; Sumpter, B. G.; Orozco, M.; Luque, F. J.; Di Felice, R.; Fuentes-Cabrera, M., Ab initio Study of the Structural, Tautomeric, Pairing, and Electronic Properties of Seleno-Derivatives of Thymine. *J Phys Chem B* **2009**, *113* (43), 14465-14472.
16. Vazquez-Mayagoitia, A.; Fuentes-Cabrera, M.; Sumpter, B. G.; Sponer, J. E., PHYS 249-Ab initio study of alternative genetic systems. *Abstr Pap Am Chem S* **2009**, 237.
17. Vazquez-Mayagoitia, A.; Fuentes-Cabrera, M.; Sumpter, B. G.; Huertas, O.; Luque, S. F. J.; Orozco, M.; Di Felice, R., PHYS 276-Ab initio investigation of naphtho and benzo homologated DNA bases and the effects of substituents. *Abstr Pap Am Chem S* **2009**, 237.
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