

## Estela Blaisten-Barojas

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Department of Computational and Data Sciences, George Mason University  
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### I. Professional Preparation

Université Pierre et Marie Curie (former Paris VI), France, Doctorat ès Sciences Physiques (PhD, 1974)  
Université de Paris VI, France, Doctorat de 3ème Cycle, Physique Moléculaire Théorique (MS, 1970)  
Universidad Tecnológica de Tucumán, Argentina, Bachelor of Science, Major in Physics (BS, 1964)

### II. Academic/Professional Appointments

2009-2010 Program Director, Chemistry Division, National Science Foundation.  
2006-present Director, Computational Materials Science Center, George Mason University, GMU.  
1992-present Professor, Department of Computational and Data Sciences, and Department of Chemistry and Biochemistry, GMU.  
1990-1992 Visiting Professor, Departments of Chemistry and Physics, Johns Hopkins University  
1988-1989 Guest Professor, Center for Fire Research & Process Measurements Division, NIST  
1987-1988 Visiting Professor, Department of Physics, Virginia Commonwealth University  
1981-1982 Visiting Professor, Department of Chemistry, Stanford University  
1981-1992 Professor, Institute of Physics, Universidad Nacional Autónoma de Mexico (UNAM)  
1978-1981 Associate Professor, Institute of Physics, UNAM  
1975-1978 Assistant Professor, Institute of Physics, UNAM

### III. Publications: 10 relevant publications with doctoral students (from a total of 110 peer-reviewed)

1. X. Dong, D. K. Klimov and E. Blaisten-Barojas, "Protein Folding with the Adaptive Tempering Monte Carlo Method," *Molecular Simulation* **33**, 577-582 (2007).
2. A. Patrick, X. Dong, T. Allison, and E. Blaisten-Barojas, "Silicon Carbide Nanostructures: a Tight Binding Approach," *J. Chem. Phys.* **130**, 244704 (2009) highlighted in *vjnano.org* 20 (1), (2009).
3. Y. Dai and E. Blaisten-Barojas, "Monte Carlo Study of Oligopyrroles in Condensed Phases," *J. Chem. Phys.* **133**, 034905 (2010).
4. D. Sponseller and E. Blaisten-Barojas, "Failure of logarithmic oscillators to serve as a thermostat for small atomic clusters," *Physical Review E* **89**, 021301(R) (2014).
5. C. Hall, W. Ji, and E. Blaisten-Barojas, "The Metropolis Monte Carlo method with CUDA enabled Graphic Processing Units," *J. Computational Physics* **258**, 871-879 (2014).
6. Y. Dai, Ch. Wei, and E. Blaisten-Barojas, "Density functional theory study of neutral and oxidized thiophene oligomers," *J. Chem. Phys.* **139**, 184905 (2013).
7. R. Massaro and E. Blaisten-Barojas, "Theoretical investigation of the photophysics of methyl salicylate isomers." *J. Chem. Phys.* **135**, 164306 (2011).
8. R. Massaro and E. Blaisten-Barojas, "Density Functional Theory Study of Dipicolinic Acid Isomers and Crystalline Polytypes." *Computational and Theoretical Chemistry* **977**, 148-156 (2011).
9. S. Yang, M. Lach-hab, I. I. Vaisman, and E. Blaisten-Barojas, E., "Identifying Zeolite Frameworks with a Machine Learning Approach," *J. Phys. Chem. C*, **113**, 21721-21725 (2009)
10. M. Lach-hab, S. Yang, I. I. Vaisman, E. Blaisten-Barojas, "Novel Approach for Clustering Zeolite Crystal Structures." *Molecular Informatics* **29**, 297-301 (2010).

### IV. Synergistic Activities

#### a) Honors and Awards:

2012-present Member Editorial Board, The Scientific World Journal: Atomic and Molecular Physics and the Journal of Theoretical Chemistry  
2006 Fellow of the American Physical Society  
2004-present Member Editorial Board, Journal of Computational & Theoretical Nanoscience  
1990-92 National Science Foundation Visiting Professorship, Johns Hopkins University

1984-present	Investigador Nacional. Award for excellence & distinguished research, Mexico
1982-1983	Fulbright Senior Fellow, Department of Chemistry, Stanford University
1983-1983	International Fellow, Educational Foundation of the AAUW
1980-present	Member of the Mexican Academy of Sciences

b) **Teaching:** Over 15 different courses developed and taught at undergraduate and graduate level. Three summer school courses in Trieste and Sicily, Italy.

**c) Organization of Events, University Leadership, and Governance Experience:**

Faculty Representative to the GMU Board of Visitors (2013-2015)

Graduate Coordinator of the Computational and Sciences Programs, GMU (2006-2013, 2015-present)

Coordinator of the Mason Nanotechnology Initiative, GMU (2004-present)

Chair, Review Committee the Edward A. Bouchet Award, American Physical Society (APS) (2012- )

Chair, Review Committee of the Nicholas Metropolis prize of the APS (2004-2006)

Member Committee of International Scientific Affairs of APS (2002-2005)

Member at Large, Executive Committee of the Division of Computational Physics, APS (2001-2004)

Member of the Executive Committee of the Faculty Senate (1997-2002)

Chair, Organization and Operations Committee of the Faculty Senate GMU (1997-2002)

Chair, Curriculum Committee School of Computational Sciences and College of Science (1996-2006)

Director of the Laboratory for Computer Design of Materials, SCS-GMU (1993-2005)

Organizer: Colloquium of the Computational Materials Science Center, GMU (1993- ); March

Meeting APS Simulation of Complex Materials Focus Session (2004 and 2005); East

Coast Symposium on the Chemistry and Physics of Clusters and Cluster Ions (1991).

Co-organizer: Meeting of the Division of Computational Physics of the APS, Austin (2003).

Chair of 9 faculty search committees; Chair of 8 promotion and tenure committees; Vice-president AAUP-GMU chapter in 1998.

d) **Presentations and Abstracts in Scientific Conferences:** Over 60 invited presentations in conferences and university colloquia, plus 170 contributed works to conferences with published abstracts.

**e) Service to the Research Community:**

- Reviewer: J. Chem. Phys., J. Phys. Chem. A, J. Phys. Chem. C, Chem Phys Lett, Comp. & Theor. Chemistry, Comp. Phys., JACS, J. Chem. Information & Modeling, Modelling Simul. Mater. Sci. Eng., Microporous & Mesoporous Materials, Crystal Growth & Design
- Proposals and panels reviewer: NSF, NASA, DOE, ORAU, ACS, VA Center Innovative Technology
- Session chair in several APS meetings, ACS meetings and in the 2002 DCOMP conference
- Member of the Advisory Board of the NSF CIRE-PUMP program, U. of Puerto Rico-Humacao
- Support participant of ADVANCE-Institutional Transformation to U. Puerto Rico-Humacao
- Member of: American Chemical Society, American Physical Society, & Materials Research Society
- NVIDIA academic research partner

**V. Collaborations**

**a) External Collaborators in the Last 48 Months:**

T. Allison (NIST), V. Barsegov (U. Massachusetts, Lowell), K. Kehn-Hall (GMU), M. Chen (WIP-Japan), S. Guharay (Mitre), D. Klimov (GMU), V. Karen (NIST), D. Klimov (GMU), X. Li (NIST), A. Mitraki (UoC, Greece), M. Pederson (NRL), J. Purton (Daresbury, UK), D. Roberts (Noblis), A. Shehu (GMU), H. Sheng (GMU), E. Smela (UMD), I. Takeuchi (UMD), I. Vaisman (GMU), W. Xi (Nanjing U., China).

**b) Thesis advisor of Graduate Students and Sponsor of Postgraduate Students:**

PhDs: Y. Li (97), M. Lach-hab (98), A. AlSunaidi (99), C. Chien (00), J. Mirick (02), G. Wang (02), X. Dong (06), A. Patrick (08), Y. Dai (09, best dissertation), J. Lyver (10), R. Massaro (11, best dissertation), C. Hall (13). PhDs in the pipeline: Y. Abere, G. Helmick, D. Reitz, D. Sponseller, MSs: S. Evans (95), J. Waltz (98), C. Cruz (00), L. Gebremedhin (04), A. Khan (07). Postdocs: Y. Dai, D. A. Carr, M. Lach-hab, S. Yang.