

Curriculum Vitae

Patricia Guadarrama Acosta



Current Position

Titular Researcher at Materials Research Institute.
National Autonomous University of Mexico (UNAM).
Apartado Postal 70-360, CU, Coyoacán, México DF
04510, México.
Phone: +(52)(55) 56224594
Fax: +(52)(55) 56161201
E-mail: patriciagua@correo.unam.mx
patyguadarrama@yahoo.com

Current Projects

- Substitution of Macrocycles-containing Heteroatoms with Dendrimeric Branches. Synthesis and Theoretical studies considering the concept of Molecular Collectivity.
- Dendrimers for molecular recognition and catalysis. Design by Computational Chemistry.
- Study of pollutant agents (chloride-compounds).

Participation in:

- Theoretical Study of Electronic Properties and Synthesis of Polymeric charge-transfer Complexes of C60 and C70. (Sponsored by CONACyT; contract number: 33631E)
- Synthesis and Molecular Simulation of Hyper-branched Polymers with Optical Properties. (Sponsored by CONACyT; contract number: 25092E).
- Theoretical Study of Formation and Behavior of Asphaltenes. (Mexican Institute of Oil. Research proposal D.00329).

Education

National Autonomous University of Mexico (UNAM). Faculty of Chemistry. **PhD in Organic Chemistry (June 2000)**. Dissertation: "Solid-supported synthesis of well-defined conjugated dendrimeric oligomers and hyper-branched polymers with optical properties". Advisor: Dr. Serguei Fomine.

National Autonomous University of Mexico (UNAM). Faculty of Chemistry. **M.Sc. in Organic Chemistry (November 1997)**. Thesis: "Synthesis, characterization and theoretical study of hyper-branched poly-unsaturated compounds". Advisor: Dr. Roberto Salcedo.

National Autonomous University of Mexico (UNAM). Faculty of Chemistry. **B.Sc. in Chemistry (June 1994)**. Thesis: "Theoretical Study about Reactivity of Enines". Advisor: Dr. Roberto Salcedo.

Research Experience

2000-2001. Post-doctoral position at Center of Molecular Design and Recognition (University of South Florida, U.S.A.). Research Topic: Synthesis and Molecular Simulation of Dendrimers. Supervisor: Dr. George Newkome.

1998 to present. Research work in Synthesis and Characterization of Hyper-branched Polymers and Dendrimers (Polymer Synthesis Lab at IIM) and Molecular Simulation using different levels of theory (Molecular Dynamics, Molecular Mechanics, Semiempirical and Ab initio methods) included in software packages like: Gaussian, Macromodel, Jaguar, etc.

2001 to present. Collaboration with Mexican Institute of Oil (Filial of Mexican Oil Company PEMEX) in Molecular Simulation of Asphaltenes.

Industrial Experience

1994-1995. Química Hoechst de México (Synthesis and Quality Control. Pigments and Dyes Division).

Teaching Experience

1998-1999. High School Teacher in Organic Chemistry. ITESM, Ciudad de México (Private School in Mexico).

2002 to present . Organic Chemistry laboratory courses (Faculty of Chemistry. National Autonomous University of Mexico (UNAM)).

2002 to present: postgraduate courses of Functional Organic Materials (Materials Research Institute (UNAM)).

Languages

Spanish (Native speaker).

English (Fluent speaker).

French (Technical translation).

Awards

1993. Annual Award “Gustavo Baz Prada” in Technology of Functional Polymers (Research developed at Materials Research Institute, UNAM, Mexico).

2000. Annual Award “Alfonso Caso” to the most distinguish PhD dissertation.

Professional Society Memberships

Member of the Mexican Society of Chemistry since 1995 to present.

Publications

1) R. Salcedo; T. Ogawa; A. Pineda; M. Rubio; M. García; P Guadarrama, *Polymer* **1992**, 33, 5300-5302. Chemical Pathways for the polymerization of enines.

2) L. E. Sansores; R. Salcedo; L. Fomina; P. Guadarrama, *J. Mol. Structure* **1997**, 389, 217-226. Electronic Structure study of planar conjugated eight-membered ring compounds.

- 3) L. Fomina; P. Guadarrama; S. Fomine; R. Salcedo; T. Ogawa, *Polymer* **1998**, 39, 2629-2635. Synthesis and characterization of well defined fully conjugated hyperbranched oligomers of β,β -dibromo-4-ethynylstyrene.
- 4) R. Salcedo; L. E. Sansores; P. Guadarrama, *J. Mol. Structure* **1998**, 430, 23-27. Stability of centrohexaindane.
- 5) S. Fomine; L. Fomina; P. Guadarrama, *Macromol. Theory Simul.* **1999**, 8, 54-60. Molecular modelling of hyperbranched polyacetylene.
- 6) P. Guadarrama; L. Fomina; V. Pankov; W. Matus; S. Fomine, *Polymer J.* **1999**, 31, 423-428. Solid-supported synthesis of hyperbranched polymer with discrete conjugated units.
- 7) S. Fomine; L. Fomina; P. Guadarrama, *J. Mol. Structure* **1999**, 488, 207-216. Electronic structure of fully conjugated dendritic oligomers of β,β -dibromo-4-ethynyl styrene.
- 8) L. Fomina; P. Ponce; P. Guadarrama; S. Fomine, *Macromol. Theory Simul.* **1999**, 8, 403-408. Effect of terminal groups on the electronic structure of hyperbranched polyacetylene.
- 9) P. Guadarrama; L. Fomina; S. Fomine, *Macromol. Theory Simul.* **2000**, 9, 263-269. Molecular modelling of solid-supported polymerisation of 4-(5-hexynyloxy)- β,β -dibromo styrene.
- 10) P. Guadarrama; L. Fomina; S. Fomine, *Polymer* **2001**, 50, 76-83. Solid-supported synthesis of hyperbranched polymer with β,β -diethynylstyryl units.
- 11) I García-Cruz; J.M. Martínez-Magadán; P. Guadarrama; R. Salcedo, F. Illas; *J. Phys. Chem. A* **2003**, 107, 1597-1603. Electronic Structure Properties of Carbazole-like Compounds: Implications for Asphaltene Formation.
- 12) S. Fomine*, L. Fomina, P. Guadarrama, *Macromol. Symp.*, **2003**, 192, 43-61. Synthesis, properties and molecular modeling of functional hyperbranched polymers and dendrimers.
- 13) P. Guadarrama*; S. Fomine; R. Salcedo, *J. Mol. Mod.*, **2003**, 9, 273-282. Cyclen substitution with urea-containing dendrimeric branches. Theoretical study considering the concept of collectivity.
- 14) A. Reyes; M. Tlenkopatchev; L. Fomina, P. Guadarrama, S. Fomine*, *J. Phys. Chem. A* **2003**, 107, 7027-7031. Local MP2 based method for estimation of intermolecular interactions in aromatic molecules. Benzene, Naphthalene and Pyrimidine dimers. A comparison with canonical MP2 method.
- 15) L. Fomina, A. Reyes, P. Guadarrama, and S. Fomine ONIOM (MP2:PM3) Study of C₆₀-water Complex. *International Journal of Quantum Chemistry*, **2004**, 97, 679-687.
- 16) Gabriela Osorio; Carlos Frontana; Patricia Guadarrama*; Bernardo A. Frontana-Uribe*, *J. Phys. Org. Chem.* **2004**, 17, 439-447. Electrochemical and Theoretical Study of a Family of Fully Conjugated Dendritic Oligomers.
- 17) Delia Soto-Castro; Patricia Guadarrama*, *J. Comput. Chem.* **2004**, 25, 1215-1226. Macrocyclic versus Dendrimeric effect. A DFT study.
- 18) Aurelio Evangelista-Lara, Patricia Guadarrama*, *Int. J. Quantum Chem.* **2005**, 103, 460-470. Theoretical Evaluation of the Nano-carrier Properties of Two Families of Functionalized-Dendrimers.
- 19) Carlos Romero, Patricia Guadarrama, Serguei Fomine*, *J. Mol. Mod.*, **2005**, **ACEPTADO**. Interactions in Molecular Switches based on Crown Ethers-secondary Ammonium Motifs. A Theoretical Study.
- 20) Jorge A. Cruz-Morales; Patricia Guadarrama Acosta*, *J. Mol. Structure*, **2005**, **ACEPTADO**. Synthesis, Characterization and Computational Modeling of Cyclen Substituted

with Dendrimeric Branches. Dendrimeric and Macrocyclic Moieties Working Together in a Collective Fashion.

21) Roberto Salcedo, Ana Martínez, Patricia Guadarrama Carlos Olvera, L. Enrique Sansores, *J. Mol. Struc. THEOCHEM* **2005**. **ACEPTADO**. A theoretical study of aromaticity in 1,2-diaza and 1,2-diphospha-cyclooctatetraenes and their role as ligands in organometallic compounds.

National Publications

19) P. Guadarrama*; S. Fomine; L. Fomina, *Boletín de la SPM*, **2003**, 2, 3-14. Síntesis, propiedades y modelado molecular de dendrímeros y polímeros hiper-ramificados conjugados.

20) Jorge Armando Cruz Morales; Patricia Guadarrama Acosta*, *Materiales Avanzados*, **2004**, 3, 19-28. Dendrímeros: Imitando a la Naturaleza.

Articles in Extenso

R. Salcedo; P. Guadarrama; L. E. Sansores; S. Fomine; L. Fomina, *Mat. Res. Soc. Symp. Proc.* **1999**, 560, 359-364. Theoretical description of luminescent effects in β,β -Di (4'-formylphenylethynyl)-4-ethynylstyrene.

Chapters in Books

S. Fomine; L. Fomina; P. Guadarrama, *Recent Advances in Macromolecules*. Global Research Network, Ed. R. Mohan Killioalam, Thiruvanthapuram 36, p.57-71, **2000** ISBN 81-87736-04-06. Synthesis, properties and molecular modeling of conjugated hyperbranched polymers and dendrimers.

Oral Presentations

1993. "Synthesis and characterization of (N₂O₂)-5,5'-substituted Schiff Bases-Ruthenium (III) compounds". XXX Mexican Congress of Chemistry (Cancún, Méx.). P. Guadarrama, R. Moreno, L. Ruíz.

1997. "Synthesis, characterization and theoretical study of hyper-branched poly unsaturated oligomers". I Student Congress at Materials Research Institute (Mexico City). P. Guadarrama, S. Fomine.

1998. "Solid-supported synthesis of well-defined dendrimeric oligomers and hyper-branched polymers". II Student Congress at Materials Research Institute (Mexico City). P. Guadarrama, S. Fomine.

1998. "Solid-supported synthesis of well-defined dendrimeric oligomers". XXXIII Mexican Congress of Chemistry (Oaxaca, Méx.). P. Guadarrama, S. Fomine.

1999. "Solid-supported synthesis of hyper-branched oligomers with discrete unsaturated units". XII National Polymer Conference (Mérida, Méx.).

2001 "Solid-Supported Synthesis of Hyperbranched Polymer with Discrete Conjugated Units". 7th Pacific Polymer Conference (Oaxaca, Méx.). P. Guadarrama, S. Fomine.

2002. "Molecular modeling of solid-supported polymerization of 4-(5-hexynyloxy)- β,β -dibromostyrene". 6th World Congress of Theoretically Oriented Chemists (Lugano, Swiss). P. Guadarrama, S. Fomine.

2003. "Cyclen substitution with urea-containing dendrimeric branches. Theoretical study considering the concept of collectivity". 8th Pacific Polymer Conference (Bangkok, Thailand). P. Guadarrama, S. Fomine, R. Salcedo.

2004. "Macrocyclic vs Dendrimeric effect. A DFT Study". International Conference of Supramolecular Science & Technology (Prague, Czech Republic). Delia Soto-Castro; Patricia Guadarrama.

Hobbies

Climbing, Jazz-Dancing, Painting and Reading.