

CURRICULUM VITAE

Vladimiro Mujica.

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CITIZENSHIP: Venezuela.

EDUCATION: Licenciado en Química, 1979.
Universidad Central de Venezuela, Caracas, Venezuela.
Thesis: "Relationships between the theory of molecular fragments and the Hohenberg-Kohn theorem".
Supervised by Dr. Eduardo Ludeña.

Ph.D., 1985, Uppsala University, Uppsala, Sweden.
Thesis: "Two broken symmetries in Quantum Chemistry: Localized excitations in two-electron ions and polyenes". Supervised by Professor Osvaldo Gosinski.

Post-Doctoral Fellow, School of Chemistry, University of Tel-Aviv, Tel-Aviv, Israel. With Professor Abraham Nitzan.

EMPLOYMENT

Academic experience:

2016: Distinguished Researcher on Sabbatical Year, Donostia International Physics Center, San Sebastian, Spain

2015: Visiting Scholar on Sabbatical Year, Department of Chemistry, Northwestern University

2011: Visiting Professor, Institute of Physics, University of Sao Paulo, Brazil

2009: Professor, Department of Chemistry and Biochemistry, Arizona State University

2008: Visiting Professor, University of Barcelona, Spain.

2006: Visiting Professor, University of Paris, Orsay, France

2005- Research Professor, Department of Chemistry
Northwestern University, Evanston, Illinois. Joint appointment with Argonne National Laboratory.

2001-2005- Senior Research Associate, Department of Chemistry
Northwestern University, Evanston, Illinois.

2004: Visiting Scholar, Korea Institute for Advanced Studies

2003: Visiting Professor, University of Marsielle, France

Curriculum Vitae Vladimiro Mujica

2004: Visiting Professor, Department of Quantum Chemistry, Uppsala University, Sweden.

2001: Visiting Professor, Department of Quantum Chemistry, Uppsala University, Sweden.

1998-2001: Visiting Professor, Department of Chemistry, Northwestern University, Evanston, Illinois.

1997- Universidad Central de Venezuela, Professor of Chemistry

1994, 1995, 1996: Visiting Scholar, Northwestern University, Evanston, Illinois.

1993: On Sabbatical leave. Northwestern University, Evanston, Illinois.

1992- Universidad Central de Venezuela, Associate Professor

1991: Invited Professor. Fritz Haber Institut, Berlin, Germany.

1989- Collaborator in the Groups of Theoretical Chemistry and Molecular Physics. Instituto Venezolano de Investigaciones Científicas.

1986-1992 Assistant Professor, Universidad Central de Venezuela.

1988: Invited Professor, Uppsala University, Sweden.

1987-1988 : Invited Professor School of Chemistry, University of Tel-Aviv.

1980-1986: Instructor Professor, Universidad Central de Venezuela. On leave in Uppsala, Sweden.

1979-1980: Instructor, Universidad Central de Venezuela.

Administrative and Service:

(2016) Member Committee of Visitors NSF, Chemistry Division

2010-present Associate Director PSM in Nanoscience, ASU

2011-present member Graduate Committee, School of Molecular Sciences, ASU

2015-present Member ASU Senate

1996-1999 Chairman of the National Commission for Oil Research, Venezuela.

1994-1995 Member of the Interamerican Committee of Science and Technology of the Organization of American States.

1994-1999 Member of the Board of Directors of the National Research Council, Venezuela.

1994-1996 Member of the Faculty Board, Facultad de Ciencias, Universidad Central de Venezuela.

Curriculum Vitae Vladimiro Mujica

1993-1997 Chairman of the Chemistry Graduate School Board
Facultad de Ciencias, Universidad Central de Venezuela.

1992-1994 Member of the Department Board, Facultad de
Ciencias, Universidad Central de Venezuela.

1988-1992 Coordinator of the Group of Theoretical Chemistry,
Facultad de Ciencias, Universidad Central de Venezuela.

1988- Member of the Chemistry Graduate School Board
Facultad de Ciencias, Universidad Central de Venezuela.

1989- Coordinator of the Research Committee
Facultad de Ciencias, Universidad Central de Venezuela.

1990-1992 Member of the Faculty Board, Facultad de
Ciencias, Universidad Central de Venezuela.

COURSES TAUGHT:

Thermodynamics (Undergraduate)

Introductory Statistical Mechanics and Chemical Kinetics
(Undergraduate).

Introductory Quantum Chemistry. (Undergraduate).

Chemical Kinetics (Graduate).

Advanced Quantum Chemistry (Graduate).

Stochastic processes (Graduate).

Molecular Spectroscopy (Graduate)

Statistical Thermodynamics (Graduate)

Assistant as undergraduate student in courses of Mathematical
Methods for Chemists, Inorganic Chemistry, Modern Physics,
Physical Chemistry and Introductory Quantum Chemistry, at the
Faculty of Sciences, Universidad Central de Venezuela, from 1977 to
1979.

PUBLICATIONS:

Articles

(1) E.Ludeña and V.Mujica
"Virial Fragments and the Hohenberg-Kohn Functional",
Int.J.Quant.Chem., 21(1982)927.

(2) V.Mujica, O.Goscinski and E.Sangfelt
"Electron Correlation in Doubly Excited States of Helium and
Extensions to Beryllium and Magnesium",
Chem.Phys., 87(1984)473.

- (3) V.Mujica, N.Correia and O.Goscinski
"Fermion-propagator Calculations of Excitations in Polyenes using a Heisenberg (XYZ) Hamiltonian, I. Formalism and Parametrization",
Phys.Rev. B 32(1985)4178.
- (4) V.Mujica, N.Correia and O.Goscinski
"Fermion-propagator Calculations of Excitations in Polyenes using a Heisenberg (XYZ) Hamiltonian, II. Applications to Large Systems",
Phys.Rev. B 32(1985)4186.
- (5) O.Goscinski and V.Mujica
"Adiabatic Coordinate Separation and Large N-dimensional Limit in Two-Electron Ions",
Int.J.Quant.Chem., 24(1986)897.(6) O.Goscinski and V.Mujica
"Adiabatic Separation, Broken Symmetries and Geometry Optimization", R.Erdahl, V.H.Smith (eds.),
"Density Matrices and Density Functionals", (1987)597,
D.Reidel Pub. Co.
- (7) V.Mujica, Y.Li and O.Goscinski
"Dynamic Coordinate Separation and State-dependent Potentials. An Analysis of Localization in Helium",
Chem.Phys. 112(1987)159.
- (8) V.Mujica
"Some Physico-Chemical Aspects of Conducting Polymers".
Proceedings of the Venezuela-Italia Workshop "Innovation and Technological Training in Polyolefins", Caracas (1989)
- (9) G. Doyen, D. Drakova, Mujica V and M. Scheffler
Theory Of The Scanning Tunneling Microscope
Phys Status Solidi A 131: (1) 107-108 May 16 1992
- (10) E.Ludeña and V.Mujica,
"Kohn-Sham Theory and N-representability".
J.Mol.Struct.(Theochem) 210(1990)9.
- (11) M.García-Sucre and V.Mujica
"Regional Virial Relations for Arbitrary Subsystems of Particles of a Molecule with Nuclear Motion Quantum Mechanically Described".
Int.J.Quantum Chem. Quantum Chemistry Symp. 24(1990)375.
- (12) B.Carmeli, V.Mujica, A.Nitzan, "Dynamics of Multidimensional Barrier Crossing in the Overdamped Limit".
Ber.Bunsenges.Phys.Chem., 95(1991)319
- (13) E.S.Kryachko, E.V.Ludeña and V.Mujica
"Toward a Non-Born-Oppenheimer Density Functional Theory".
Invited contribution to the International Workshop on Condensed Matter Theories, Italy, June 1990. Condensed Matter Theories, S.Fantoni, S.Rosati (eds.), Plenum Press (1991) New York.

- (14) V.Mujica, "Some Theoretical Aspects of Electroactive Polymers". Invited conference to the International Symposium on Applied Theoretical Chemistry, Havana, Cuba, Julio 1990.
"Trends in Applied Theoretical Chemistry", L.A.Montero, Y.G.Smeyers (eds.), Kluwer Academic Publishers, Dordrecht (1992).
- (15) E.S.Kryachko, E.V.Ludeña and V.Mujica
"Non-Born-Oppenheimer Density Functional Theory".
Int.J.Quantum Chem., 40(1991)589.
- (16) V.Mujica, M.García Sucre and Y.Aray
"Regional Virial in Diatomic Molecules. Two criteria for defining zero-flux dividing surfaces".
J.Mol.Struct., Theochem. 254(1992)125.
- (17) E.S.Kryachko, E.V.Ludeña and V.Mujica
"Density Functional Theory in the Context of Local-Scaling Transformations and its Prospects for Applications in Catalysis".
"Quantum Chemistry Approaches to Chemisorption and Heterogeneous Catalysis", F.Ruette (ed.), Kluwer Academic Publishers, Dordrecht (1992).
- (18) G. Sánchez, Z.Brito, G.Perdomo and V.Mujica.
"The Thermal Behavior of Cured Epoxy-Resins. The Influence of Metallic Fillers."
Polymer Degradation and Stability 40(1992)109
- (19) V.Mujica, and G.Doyen.
A Green's Function Calculation of the Zero-Voltage STM Resistance of a One-Dimensional Chain Coupled to Two Jellium Surfaces"
Int. J. Quantum Chem. Suppl. 27(1993)687.
- (20) M. García Sucre, J. L. Paz, E. Squitieri, and V. Mujica.
"Intramolecular Coupling Effect in the Refractive Index for a Simple Three-Level Model of Molecules Diluted in Water"
Int. J. Quantum Chem. Symp. 27(1993)699.
- (21) E. Squitieri, M. García Sucre, J. L. Paz, and V. Mujica
"The Effect of Vibronic Coupling on the First and Second Order Electric Susceptibility in a Simple Model of a Molecule"
Optica pura y aplicada, 26(1993)195.
- (22) J. L. Paz, M. García Sucre, E. Squitieri, and V.Mujica
"The Effect of Intramolecular Coupling on the Optical Susceptibilities of a two-level molecule"
Chemical Phys. Lett. 217(1994)333-341.
- (23) V.Mujica, M.Kemp and M.Ratner
"Effect of Disorder on the STM Current of a One-Dimensional Chain"
Abstracts of Papers of the American Chemical Society, 1993, Vol. 206, Iss August, pp 134-PHYS.

- (24) M.Kemp, V.Mujica and M.Ratner
"Effect of Dimensionality on the STM current of Disordered Molecular Systems"
Abstracts of Papers of the American Chemical Society, 1993, Vol. 206, Iss August, pp 135-PHYS.
- (25) A.Cheong, A.Roitberg, V.Mujica and M.Ratner
"Resonances and Interference Effects on the Effective Electronic Coupling in Electron Transfer"
J.Photochem. and Photobio. A: Chem., 82(1994)81-86.
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"Refractive index in a dilute solution of molecules with intramolecular coupling up to third order in the external field"
Mol. Phys. 82(1994)227.
- (27) M.García Sucre, E.Squitieri, J.L.Paz and V.Mujica
"Absorptive and dispersive processes in a two-level molecule with intramolecular coupling and non-zero permanent dipole moment"
J.Phys. B, 27(1994)4945-4972
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"Electron Conduction in Molecular Wires. (I) A Scattering Formalism".
J. Chem. Phys. 101(1994)6849-6855.
- (29) V.Mujica, M. Kemp and M. A. Ratner
"Electron Conduction in Molecular Wires. (II) Applications".
J. Chem. Phys. 101(1994)6856-6864.
- (30) M.Kemp, V.Mujica and M.Ratner
"Molecular Electronics: Disordered Molecular Wires".
J. Chem. Phys. 101(1994)5172-5178.
- (31) V.Mujica.
"STM Molecular Imaging of Disordered Molecular Wires"
In: "Surfactants in Solution", A.Chattopadhyay and K.L.Mittal (eds.).
Marcel Dekker, Inc. New York (1996).
- (32) M.Kemp, A. Roitberg, V.Mujica, T.Wanta and M.A.Ratner
"Molecular wires: Extended couplings and disorder effects".
J. Phys. Chem., 100(1996)8349-8355
- (33) V. Mujica, M.Kemp, A.Roitberg and M.A.Ratner
"Current-Voltage characteristics of molecular wires. Eigenvalue staircase, Coulomb blockade, and rectification"
J. Chem. Phys., 104(1996)7296-7305.
- (34) V.Mujica, M.Kemp, A.Roitberg and M.A.Ratner
"A model for Coulomb interaction in electron transport in one-dimensional mesoscopic devices".
In: *Condensed Matter Theories 11* . E.V. Ludeña, P.Vashishta and R.F. Bishop (eds.), Nova Science Publishers, Commack, N.Y. (1996).

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"Applications of photothermal displacement spectroscopy to the study of asphaltene adsorption"
Optics Communications 145,(1997)69-75.
- (36) M. Kemp, V. Mujica, A. Roitberg, Y. Mao and M. A. Ratner
"Molecular wires: Resonances, staircases, rectification, bonding and speculation".
In: *Atomic and Molecular Wires*. C. Joachim and S. Roth (eds.), Kluwer Academic Publishers. The Netherlands (1997).
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"Electron transfer rates in bridged molecular systems: A phenomenological approach to relaxation".
J. Phys. Chem. A, 101(1997)6158-6164.
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"A conformational study of the influence of vibrations on electronic conduction in molecular wires".
J. Phys. Chem. B, 102(1998)941-947.
- (39) V. Mujica, and M. Kemp
"Electron transfer and molecular conductance: Similarities, differences and continua"
Abstracts of Papers of the American Chemical Society, 1998, Vol. 215, Iss March, pp 289-PHYS.
- (40) A. Roitberg, V. Mujica and M.A. Ratner
"Molecular wires: Computation of the conductance decay length"
Abstracts of Papers of the American Chemical Society, 1998, Vol. 215, Iss March, pp 290-PHYS.
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"Molecular wires: Charge Transport, Mechanisms and Control".
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"Application of photothermal spectroscopy to water-surfactant systems near CMC"
Mikrochimica Acta 130(1998)105.
- (43) M. Kemp, V. Mujica and M. A. Ratner
"Molecular Wire Interconnects: Chemical Structural Control, Resonant Tunneling and Length Dependence" *VLSI Design*, vol. 8, no. 1-4 , pp. 65-74, 1998. doi: 10.1155/1998/73516
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"Electron transfer in molecules and molecular wires: Geometry dependence, coherent transfer and control".
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"A semi-empirical quantum chemical study of some local aspects of ionic conduction in poly(ethylene oxide): Ion motion and rotational barriers".
Journal of Physical Chemistry A 103(1999)89.
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"Non Born-Oppenheimer corrections in an exactly solvable model of the hydrogen ion molecule".
Journal of Physics B At. Mol. 31(1998)4537.
- (47) Natalia León, Pedro Nieto and Vladimiro Mujica
"Estimación del tiempo de residencia de un electrón en un alambre molecular"
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- (48) S.N.Yaliraki, A.E.Roitberg, C.González, V.Mujica and M.A.Ratner
"The injecting energy at molecule/metal interfaces: implications for conductance of molecular junctions from an *ab initio* molecular description".
J. Chem. Phys. 111(1999)6997.
- (49) J. Castillo, J. Hung, A. Fernández and V. Mujica
"Nonlinear Optical Effects in Asphaltene Solutions", in Power-Limiting Materials and Devices. Christopher M. Lawson, Editor, Proceedings of SPIE 3789 (1999) 148-154.
- (50) V. Mujica, E. Squitieri and P. Nieto
"Generalized virial partitions and the one-particle density matrix".
J Mol Struc-Theochem 501(2000)115-123.
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"Molecular wire conductance: Electrostatic potential spatial profile".
J. Chem. Phys. 112(2000)6834.
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"Caging of Molecules by Asphaltenes. A Model for Free Radical Preservation In Crude Oils Based on Intermolecular Energies of PAH"
Energy and Fuel 14(2000)632.
- (53)V. Mujica , C. Mina , and M. A. Ratner
Bond breaking and molecular conductance.
ABSTR PAP AM CHEM S 220: U213-U213 Part 2 AUG 20 2000
- (54)Mujica V, Ratner MA, Nitzan A
Molecular interconnects: Bridge building for charges.
ABSTR PAP AM CHEM S 220: U233-U233 Part 2 AUG 20 2000

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“Evidences of asphaltene aggregation in non linear response of solutions”.
Fuel 80 (2001) 1239.
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“Molecular Wires As Mesoscopic Systems: Similarities and Some Important Differences”.
Rev. Mex. Fis. 47 (2001) 59 Suppl. 1
- (57) V. Mujica and M. A. Ratner
“Current-Voltage characteristics of tunneling molecular junctions for off-resonance injection”.
Chem. Phys. 264 (2001) 365.
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“Correlating Electron Transport and Molecular Structure in Organic Thin Films”.
Angew. Chem. Int. Edit. 40 (2001) 2316.
- (59) Vladimiro Mujica, and Mark A. Ratner
Injection issues at molecular solid interfaces: Potential fields, disorder, and binding.
Abstr. Pap. Am. Chem. S 222: 79-Coll Part 1 Aug 2001
- (60) Vladimiro Mujica, Abraham Nitzan and Mark A. Ratner
“Molecular Rectification: Why is it so rare”.
Chem. Phys. 281 (2002) 147.
- (61) T. Cusati, J. L. Paz, E. Squitieri, M.C. Salazar, A.J. Hernandez and V. Mujica
“Four-Wave Mixing Spectroscopy Of A Two-Level System With Intramolecular Coupling. The Effect Of Relaxation Times”. Mol Phys 100(2002)1587.
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“Modeling The Electrostatic Potential Spatial Profile Of Molecular Junctions. The Influence Of Defects And Weak Links”.
Ann NY Acad Sci 960(2002)163.
- (63) Vladimiro Mujica, Osvaldo Goscinski and M. A. Ratner
“The role of electronic correlation in coherent mesoscopic transport”.
Int. J. Quantum Chem. 90 (2002) 14.
- (64) Michael L. Chabinyc, Xiaoxi Chen, R. Erik Holmlin, Heiko Jacobs, Hjalti Skulason, C. Daniel Frisbie, Vladimiro Mujica, Mark A. Ratner, Maria Anita Rampi, and George M. Whitesides
“Molecular Rectification in Self-Assembled Monolayer Junctions”
J. Am. Chem. Soc. 124 (2002) 11730
- (65) Aileen Loszán, Pedro Nieto, Sócrates Acevedo, and Vladimiro Mujica
“A Spin Polarization Transfer Approach to Intermolecular Interactions Between Hydrocarbon Aromatic Compounds and Free Radicals”.
J. Phys. Chem. A 106 (2002) 10374

- (66) Arne Keller, Osman Atabek, Mark Ratner and Vladimiro Mujica
“Laser-assisted conductance of molecular wires”
J. Phys. B: At. Mol. Opt. Phys. 35 (2002) 4981
- (67) Vladimiro Mujica and Mark A. Ratner
"Molecular Conductance Junctions: A Theory and Modeling Progress Report."
Handbook of Nanoscience, Engineering, and Technology, W. A. Goddard, III, D.
W. Brenner, S. E. Lyshevski and G. J. Iafrate (eds) (CRC Press, New York 2003).
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P. Kubiak.
“Molecular Wire Junctions: Tuning The Conductance”.
J. Phys. Chem. B 107 (2003) 91.
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“Inclusion of non-orthogonality on the valence bond charge transfer model for
nonlinear optical properties of push-pull molecules”
Mol. Phys., 101 (2003) 1805.
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Manuel Caetano
“SHG of ultrathin films of metal porphyrins on BK7 glass in total internal
reflection geometry: Theory and Experiments”
J. Phys. Chem. B 107 (2003) 9332.
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“A simple theoretical model to study the voltage dependence of the electronic
structure of phenyl ethylene oligomers”
Ann. NY Acad. Sci. 1006 (2003) 68.
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“Entangled electronic state via an interacting quantum dot”
Europhys. Lett., 66 (2004) 624.
- (73) I. Urdaneta, A. Keller, O. Atabek and V. Mujica
“Laser-assisted conductance of molecular wires. Two-photon Contribution”
Int. J. Quantum Chem. 99 (2004) 460.
- (74) C. Gonzalez, Y. Simón-Manso, J. Batteas, M. Marquez, M. A. Ratner and
V. Mujica
“A quasi-molecular approach to the conductance of molecule-metal junctions:
Theory and application to voltage-induced conductance switching”
J. Phys. Chem. B 108 (2004) 18414.
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“Current and Noise in a model of an alternating current scanning tunneling
microscope molecule-metal junction”
J. Chem. Phys., 122 (2005) 144703.
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“A simple model for laser-electrode interaction and its role in photo-assisted
electron transport processes in molecular interfaces.”
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- “Chemisorption-induced Spin Symmetry Breaking in Gold Clusters and the Onset of Magnetism in Capped Gold Nanoparticles”
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- (80) V. Mujica, T. Hansen and M. Ratner
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“A Density Functional Study of Magnetism in Bare Gold Nano-Clusters”
Phys. Rev. B **75**, 144421 (2007)
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J. Chem. Phys. 126 (2007) 161103.
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Phys. Rev. B, 76 (2007) 224409.
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“Laser-induced Nonlinear Response in Photoassisted Resonant Electronic Transport”
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“Non-adiabatic effects in electron tunneling in molecular junctions”
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“Dipole Orientation and Surface Cluster Size Effects on Chemisorption-Induced Magnetism: A DFT Study of the Interaction Gold-Thiopolypeptide”
J. Phys. Chem. A 112 (2008) 9771.
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J. Chem. Phys. 131 (2009) 014707.
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“Gold-Coated Cementite Nanoparticles: An Oxidation-Resistant Alternative to Alpha-Iron”
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J. Phys. Chem. C 114 (2010) 14642.
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J. Phys. Chem. C 114 (2010) 20870.
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“Tribute to Mark Ratner”
J. Phys. Chem. B 114 (2010) 20293.
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“Quantum Confinement Effects on the Surface Enhanced Raman Spectra of Hybrid Systems Molecule-TiO₂ Nanoparticles”
Int. J. Quantum Chem. Sp. Iss. 111 (2011) 1659.

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Oxide Nature, Size, Solvent, and pH Effects”
J. Phys. Chem. C 115 (2011) 8994.

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Exciton Transport in the FMO complex”.
J. Chem. Phys. 135 (2011) 075102

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Mujica
“Stability and Quenching of Plasmon Resonance Absorption in Magnetic Gold
Nanoparticles”
J. Phys. Chem. Lett. 2 (2011) 2996.

(102) Angelo Di Bernardo, Pilarisetty Tarakeshwar; Vladimiro Mujica
“Electronic and Vibrational Properties of magnetic core-shell nanoparticles”
Proceedings of the 6 th European Conference on Antennas and Propagation,
EuCAP 2012. 199-202 (2012)

(103) Ernesto Medina, Floralba López, Mark A. Ratner and Vladimiro Mujica
“Chiral Molecular Films as Electron Polarizers and Polarization Modulators”
EPL, 99 (2012) 17006

(104) Dalvin D. Méndez-Hernández, Pilarisetty Tarakeshwar, Devens Gust,
Thomas A. Moore, Ana L. Moore, and Vladimiro Mujica
“Simple and accurate correlation of experimental redox potentials and DFT-
calculated HOMO/LUMO energies of polycyclic aromatic hydrocarbons”
J Mol Model DOI 10.1007/s00894-012-1694-7 (2012)

(105) Héctor Franco, Luis Puerta, Juan Murgich and Vladimiro Mujica
“Simulation of Adsorption on Surfaces from ab initio Calculations on Clusters
of nanogold atoms”
Rev. Mex. Física, 58 (2012) 317.

(106) L Puerta, M Lozada, HL Sánchez, HJ Franco, C Gonzalez, V Mujica
“A Computational Analysis of Non-Covalente Interactions Between Aromatic
Compounds”
J. Comput. Meth. Sci. Eng. 12 (2012) 353-359

(107) Finkelstein-Shapiro, Daniel; Petrosko, Sarah; Dimitrijevic, Nada;
Gosztola, David; Gray, Kimberly A.; Rajh, Tijana; Tarakeshwar, Pilarisetty;
Mujica, Vladimiro
"CO₂ Pre-activation in Photo-induced Reduction Via Surface Functionalization
of TiO₂ Nanoparticles"
J. Phys. Chem. Lett. 4 (2013) 475-479

(108) Elad Mentovich, Natalie Shraga, Itsik Kalifa, Michael Gozin, Vladimiro
Mujica, Thorsten Hansen, and Shachar Richter
“Gate-controlled Rectification Behavior of a Ferrocene Self-assembled
Monolayer-based Transistor”
J. Phys. Chem. C 117 (2013), 8468-8474

- (109) Rosenberg, Richard; Symonds, Joshua; Kalyanaraman, Vijayalakshmi; Markus, Tal; Orlando, Thomas; Naaman, Ron; Medina, Ernesto; López, Floralba; Mujica, Vladimiro
"Kinetic Energy Dependence of Spin Filtering of Electrons Transmitted Through Organized Layers of DNA"
J. Phys. Chem. C 117 (2013), 22307-22313
- (110) Sharani Roy, Vladimiro Mujica, and Mark A. Ratner
"Chemistry at Molecular Junctions: Rotations and Dissociation of O₂ on the Ag(110) Surface Induced by a Scanning Tunneling Microscope"
J. Chem. Phys. 139 (2013), 074702
- (111) KS Krishna, P Tarakeswar, V Mujica, CSSR Kumar
"Chemically Induced Magnetism in Atomically Precise Gold Clusters"
Small 10 (2014) 907.
- (112) A Gunawan, CH Lin, DA Buttry, V Mujica, RA Taylor, RS Prasher, PE Phelan
"Liquid Thermoelectrics: Review of Recent and Limited New Data of Thermogalvanic Cell Experiments"
Nanoscale and Microscale Thermophysical Engineering 17 (2013), 304-323
- (113) S. Varela, E. Medina, F. López and V. Mujica
"Inelastic Electron Scattering From a Helicoidal Potential: Transverse Polarization and the Structure Factor in the Single Scattering Approximation"
J. Phys: Cond. Matte. 26 (2014) 015008
- (114) Jackson D. Megiatto, Jr., Dalvin D. Méndez-Hernández, Marely E. Tejada- Ferrari, Anne- Lucie Teillout, Oleg G. Poluektov, Tijana Rajh, Vladimiro Mujica, Thomas L. Groy, Devens Gust, Thomas A. Moore and Ana L. Moore
"A bioinspired construct that mimics radical interactions of the Tyr- His pairs of photosystem II "
Nature Chemistry 6 (2014) 423-428
- (115) Urdaneta, Ines; Pilmé, Julien; Keller, Arne; Atabek, Osman; Tarakeswar, Pilarisety; Mujica, Vladimiro; Calatayud, Monica
"Probing Raman Enhancement in a Dopamine-Ti₂O₄ Hybrid Using Stretched Molecular Geometries"
J. Phys. Chem. A 118 (2014) 1196
- (116) Tarakeswar, Pilarisetty; Palma, Julio; Finkelstein-Shapiro, Daniel; Keller, Arne; Urdaneta, Ines; Calatayud, Monica; Atabek, Osman; Mujica, Vladimiro
"SERS as a Probe of Charge-transfer Pathways in Hybrid Dye/Molecule-metal Oxide Complexes"
J. Phys. Chem. C 118 (2014) 3774
- (117) Urdaneta, Ines; Keller, Arne; Atabek, Osman; Palma Julio; Finkelstein-Shapiro Daniel; Tarakeswar, Pilarisety; Mujica, Vladimiro; Calatayud, Monica
"Dopamine Adsorption on TiO₂ Anatase Surfaces"
J. Phys. Chem. C 118 (2014) 20688

- (118) Andrey Gunawan, Hechao Li, Chao-Han Lin, Daniel A Buttry, Vladimiro Mujica, Robert A Taylor, Ravi S.Prasher, and Patrick E Phelan
“The amplifying effect of natural convection on power generation of thermogalvanic cells”
Int. J. Heat and Mass Transfer, 78 (2014) 423-434
- (119) Roy, Souvik; Mazinani, Shobeir K. S., Groy, Thomas L., Gan, Lu, Tarakeshwar, Pilarisetty, Mujica, Vladimiro, and Jones, Anne K.
“Catalytic Hydrogen Evolution by Fe(II) Carbonyls Featuring a Dithiolate and a Chelating Phosphine”
Inorg. Chem. 53 (2014) 8919-8929
- (120) Limin Xiang, Julio Palma, Christopher Bruot, Vladimiro Mujica, Mark Ratner, and Nongjian Tao
“Evidence of Intermediate Tunneling-hopping Transport Regime in DNA charge transport”
Nature Chemistry, 7 (2015) 221-226
- (121) RV Meidanshahi, SKS Mazinani, V Mujica, and P Tarakeshwar
“Electronic transport across hydrogen bonds in organic electronics”
International Journal of Nanotechnology 12 (2015) 297-312
- (122) Ernesto Medina, Luis A González-Arraga, Daniel Finkelstein-Shapiro, Bertrand Berche, Vladimiro Mujica
“Continuum model for chiral induced spin selectivity in helical molecules”
arXiv preprint arXiv:1501.06201
- (123) D Finkelstein-Shapiro, I Urdaneta, M Calatayud, O Atabek, V Mujica, and A. Keller
“Fano-Liouville Spectral Signatures in Open Quantum Systems”
arXiv preprint arXiv:1503.03051
- (124) Lu Gan, Thomas L Groy, Pilarisetty Tarakeshwar, Shobeir KS Mazinani, Jason Shearer, Vladimiro Mujica, Anne K Jones,
A Nickel Phosphine Complex as a Fast and Efficient Hydrogen Production Catalyst
J. Am. Chem. Soc. 137 (2015) 1109-1115.
- (125) Ernesto Medina, Luis A González-Arraga, Daniel Finkelstein-Shapiro, Bertrand Berche, Vladimiro Mujica
“Continuum model for chiral induced spin selectivity in helical molecules”
J. Chem. Phys. 142 (2015) 194308
- (126) I. Carmeli, M. Cohen, O. Heifler, Y. Lilach, Z. Zalevsky, V. Mujica and S. Richter
“Spatial modulation of light transmission through a single microcavity by coupling of photosynthetic complex excitations to surface plasmons”
Nat. Comm. 6 (2015) 7334
- (127) Christopher Bruot, Julio L. Palma, Limin Xiang, Vladimiro Mujica, Mark A. Ratner, and Nongjian Tao
“Piezoresistivity in single DNA molecules”
Nature Comm. 6 (2015) 8032

- (128) Vladimiro Mujica
“Nano-plasmonics: Chirality Transfer takes a jump”
Nature Chem. 7 (2015) 543-544
- (129) Dalvin D. Mendez-Hernandez, Jason G. Gilmore, Luis A. Montano, Devens Gust, Thomas A. Moore, Vladimiro Mujica
“Building and testing correlations for the estimation of one-electron reduction potentials of a diverse set of organic molecules”
J. Phys. Org. Chem. 28 (2015) 320-328
- (130) Andrey Gunawan, Pilarisetty Tarakeshwar, Daniel A Buttry, Vladimiro Mujica, Patrick E Phelan
“Improving Seebeck Coefficient of Thermogalvanic Cells Using Polyelectrolytes”
Meeting Abstract, Electrochemical Society 42 (2015) 2242
- (131) Katla Sai Krishna, Jing Liu, Pilarisetty Tarakeshwar, Vladimiro Mujica, James J Spivey, Challa SSR Kumar
“Atomically precise gold catalysis”
Royal Society of Chemistry, Catalysis Series 22 (2015) 87-122
- (132) Daniel Finkelstein-Shapiro, Monica Calatayud, Osman Atabek, Vladimiro Mujica, Arne Keller
“Non-linear Fano Interferences in Open Quantum Systems: an Exact Solution”
arXiv preprint arXiv:1509.04653
- (133) Limin Xiang, Julio Palma, Christopher Bruot, Vladimiro Mujica, Mark A Ratner, Nongjian Tao
“(Invited) Intermediate Tunnelling-Hopping Regime in DNA Charge Transport”
Meeting Abstracts, The Electrochemical Society, 40 (2015) 1644
- (134) Daniel Finkelstein-Shapiro, Inés Urdaneta, Monica Calatayud, Osman Atabek, Vladimiro Mujica, Arne Keller
“Fano-Liouville Spectral Signatures in Open Quantum Systems”
Phys. Rev. Lett. 115 (2015) 113006
- (135) Daniel Finkelstein-Shapiro, Monica Calatayud, Osman Atabek, Vladimiro Mujica, Arne Keller
“Nonlinear Fano Interferences in Open Quantum Systems: An Exactly Solvable Model”
Phys. Rev. A 93 (2016) 063414
- (136) Solmar Varela, Vladimiro Mujica, Ernesto Medina
“Effective Spin-Orbit Couplings in an Analytical Tight-Binding Model of DNA: Spin Filtering and Chiral Spin Transport”
Phys. Rev. B 93 (2016) 155436
- (137) Limin Xiang, Thomas Hines, Julio L Palma, Xuefeng Lu, Vladimiro Mujica, Mark A Ratner, Gang Zhou, Nongjian Tao
“Non-exponential Length Dependence of Conductance in Iodide-Terminated Oligothiophene Single-Molecule Tunneling Junctions”
JACS 138 (2016) 679

(138) Yoelvis Orozco–Gonzalez, Pilarisetty Tarakeshwar, Sylvio Canuto, Vladimiro Mujica

“Solvent Effects on the Dynamic Polarizability and Raman Response of Molecule-Metal Oxide Hybrid Clusters “
ChemPhysChem 17 (2016) 1-7.

(139) Micah Wimmer, Julio L Palma, Pilarisetty Tarakeshwar, Vladimiro, Mujica

“Single-Molecule Conductance Through Hydrogen Bonds: The Role of Resonances” J. Phys. Chem. Lett. 7 (2016) 2977.

(140) Shobeir K. S. Mazinani, Reza Vatan Meidanshahi, Julio L. Palma, Pilarisetty Tarakeshwar, Thorsten Hansen, Mark A. Ratner and Vladimiro Mujica

“Polarizability as a Molecular Descriptor for Conductance in Organic Molecular Circuits” J. Phys. Chem. C 120(2016) 26054.

(141) Albert C Aragonès, Ernesto Medina, Miriam Ferrer–Huerta, Nuria Gimeno, Meritxell Teixidó, Julio L Palma, Nongjian Tao, Jesus M Ugalde, Ernest Giralt, Ismael Díez–Pérez, Vladimiro Mujica

“Measuring the Spin Polarization Power of a Single Chiral Molecule” Small xx(2016)xxx.

(142) Poonam Singh, Joseph H Rheinhardt, Jarred Z Olson, Pilarisetty Tarakeshwar, Vladimiro Mujica, Daniel A Buttry

“Electrochemical Capture and Release of Carbon Dioxide using a Disulfide-Thiocarbonate Redox Cycle”
J. Am. Chem. Soc. xx(2017)xxx.

Citation indices	All	Since 2012
Citations	5094	1600
h-index	31	22
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Monographs presented as promotion works:

(1) "Separación dinámica de coordenadas y potenciales dependientes del estado: Localización en Helio y un Teorema generalizado de Hellmann-Feynman". (Dynamical separation of coordinates and state-dependent potentials: Localization in Helium and a generalized Hellmann-Feynman theorem)
Facultad de Ciencias,
Universidad Central de Venezuela (1986).

(2) "Difusión multidimensional y procesos activados en fase condensada: Tratamiento exacto y aproximaciones auto-consistentes". (Multidimensional diffusion and activated processes in condensed phase: Exact treatment and self-consistent approximations).
Facultad de Ciencias, Universidad Central de Venezuela (1988).

(3) "Relaciones viriales regionales en moléculas con movimiento nuclear descrito cuánticamente. Aplicaciones a sistemas simples" (Regional virial relationships in molecules with nuclear motion described quantum mechanically).

Facultad de Ciencias, Universidad Central de Venezuela (1992).

(4) "Conducción en dispositivos mesoscópicos"

(Conduction in mesoscopic devices).

Facultad de Ciencias, Universidad Central de Venezuela (1997).

Popularizing articles

(1) V.Mujica

"Algunas reflexiones sobre la enseñanza de la química en Venezuela", Revista de la Sociedad Venezolana de Química" (1986)

(2) V.Mujica

"Ciencia y Sociedad en el mundo contemporáneo: Desde la Química", Invited Conference in the cycle: "Ciencia y Sociedad en el mundo contemporáneo", Universidad Nacional Experimental del Táchira, San Cristóbal, Venezuela, April (1990).

RESEARCH INTEREST:

Theoretical Chemistry.

Current research activities:

- Molecular conductance. Electron transport in mesoscopic devices. Molecular electronics. Electron transfer theory and applications to chemical and biological Systems.

- Use of quantum-mechanical effective operators, their construction by means of group theoretical techniques. Collective degree of freedom in atomic and molecular systems.

- Density matrices and density functionals. Information theory. Non-adiabatic processes in molecular physics and quantum optics.

- Theory of stochastic processes applied to chemical reactions and solvent effects. Conducting polymers. Energy transfer in condensed phase.

- Non linear optics and plasmonics. Solar energy.

- Density functional theory.

PARTICIPATION IN INTERNATIONAL SCIENTIFIC EVENTS:

Invited conferences

1984: Latin-American School of Theoretical Chemistry, Caracas, Venezuela.

1990: International Symposium on Applied Theoretical Chemistry, Havana, Cuba.

1993: Wolfsberg Conference, Irvine, California, U.S.A.

Curriculum Vitae Vladimiro Mujica

- 1994: 10th International Symposium on Surfactants in Solution. Caracas, Venezuela.
- 1995: 19th International Workshop on Condensed Matter Theories, Caracas, Venezuela.
- 1996: III Congreso Venezolano de Química, Caracas, Venezuela.
- 1997: I Congreso Internacional de Optica y Fotónica, Caracas, Venezuela.
- 1998: XIV Simposio Latinoamericano de Física del Estado Sólido, Oaxaca, México.
- 1998: 215th National Meeting of the American Chemical Society, Dallas, U.S.A.
- 1998: VIII Jornadas Científicas Nacionales de la Facultad Experimental de Ciencias, Maracaibo, Venezuela.
- 1998: Gordon Research Conference on Electron Donor Acceptor Interactions. Newport, Rhode Island, U.S.A.
- 1998: XXIV Congreso Internacional de Químicos Teóricos de Expresión Latina, Puebla, México.
- 1998: Electron Transmission through molecules and molecular interfaces. Research Workshop of the Israel Science Foundation. Maagan, Israel.
- 1999: XV Latin-American Symposium on Solid State Physics, Cartagena, Colombia.
- 1999: X Simpósio Brasileiro de Química Teórica, Caxambú, Brasil.
- 2000: Fifth European Workshop on Quantum Systems in Chemistry and Physics, Uppsala, Sweden.
- 2000: Gordon Research Conference on Electron Donor Acceptor Interactions. Newport, Rhode Island, U.S.A.
- 2000: American Chemical Society Meeting, Washington, D.C., U.S.A.
- 2001: III Venezuelan Congress of Physics, Caracas, Venezuela.
- 2002: Sixth Multi-Conference on Systemics, Cybernetics and Information. Symposium on Molecular-Scale Devices. Orlando, Florida. U.S.A.
- 2002: Workshop on Molecular Wires and Devices, Laramie, Wyoming, U.S.A.
- 2002: Gordon Research Conference on Electron Donor Acceptor Interactions. Newport, Rhode Island, U.S.A.
- 2002: IX International Summer School Nicolas Cabrera, Madrid, España.
- 2003: Symposium on Molecular Materials, L'Azohia, España,
- 2003: Summer School on Chemical Reactions and Dynamics, Copenhagen, Denmark.
- 2004: OPTILAS Conference, Margarita, Venezuela.
- 2004: Invited series of Lectures on Molecular Electronics. Korea Institute for Advance Study, Seoul, and Pohang University, Korea.

Curriculum Vitae Vladimiro Mujica

- 2005: Molecular and Nanoelectronics, Current Trends and Perspectives, November 11-12, Korea Institute for Advance Study, Seoul, Korea.
- 2005: PacifiChem, Honolulu, Hawaii.
- 2006: Gordon Research Conference in Electrochemistry, Buellton, CA.
- 2006 Gordon Research Conference on Electron Donor Acceptor Interactions, Newport, Rhode Island.
- 2007 NSF Workshop, "Building Electrical Function into Nanoscale Molecular Architectures. Ballston, Virginia.
- 2007 Workshop on Molecular Conduction, Purdue University, West Lafayette, Indiana.
- 2007 Trends in Nanotechnology, San Sebastian, Spain.
- 2007 ICCMSE, Corfu, Greece.
- 2008: ACTC, Northwestern University, Evanston, U.S.A
2008. Nanotechnology and Nanoscience Workshop, 50th Anniversary Facultad de Ciencias, Universidad Central de Venezuela, Caracas, Venezuela.
- 2008: Symposium on Resonances, Technion, Haifa, Israel.
- 2009: XIII International Congress of Quantum Chemistry, Helsinki, Finland.
- 2010: Nanotechnology and Nanoscience Workshop, 52th Anniversary Facultad de Ciencias, Universidad Central de Venezuela, Caracas, Venezuela.
- 2010: III Congress on Theoretical and Computational Physical Chemistry, IVIC, Caracas, Venezuela.
- 2010: Jornadas de Investigación, Conferencia Central, Universidad de Carabobo, Valencia, Venezuela.
- 2010: Telluride Science research Center Workshop "Electronic and Magnetic Properties of Chiral Structures and their Assemblies", Telluride, CO, USA.
- 2010: Löwdin Lectures 2010, Uppsala University, Uppsala, Sweden.
- 2011: Nano and Giga Challenges in Electronics, Photonics and Renewable Energy Symposium and Summer School (Tutorial Lectures)
Moscow - Zelenograd, Russia, September 12-16, 2011
- 2011: Telluride Science Research Center Workshop . Quantum Transport in Nanoscale Molecular Systems, Telluride, CO, USA.
- 2011: Ninth Triennial Congress of the World Association of Computational and Theoretical Chemists, July 17-22, Santiago de Compostela, Spain
- 2012: "Summer Talks in Santiago III: Recent Developments in Quantum Chemistry" honoring Peter Politzer. January 9-13, Santiago de Chile, Chile.
- 2012: Sanibel Symposium, February 19-24, St. Simons Island, GA, U.S.A
- 2012: Jornadas de Investigación, Facultad de Ciencias, Universidad Central de Venezuela.

Curriculum Vitae Vladimiro Mujica

2012: EuCAP 2012, March 26-30, Prague, Czech Republic.

2012: Telluride Science Research Center Workshop “Electronic and Magnetic Properties of Chiral Structures and their Assemblies”, June 26-30, Telluride, CO, USA.

2012: 7th International Meeting on Photodynamics, Maresias, SP, Brazil

2013: ESPM VII, Electronic Structure and Processes at Molecular based Interfaces- the 7th Edition. Weizmann Institute of Science, Rehovot, Israel

2013: Telluride Science Research Center Workshop . Quantum Transport in Nanoscale Molecular Systems, Telluride, CO, USA.

2013: West Virginia University NanoSAFE Bioelectronics and Biosensing Symposium (April 2013). Charge Transfer at the Bio-inorganic Interface.

2013: XXXIX International Conference of Theoretical Chemists of Latin Expression, Quitel, Granada, Spain.

2013: Army Research Office Workshop on “Surface Plasmons, Metamaterials and Catalysis”, Rice University, Houston, Texas, U.S.A

2013: Summer School on Photo physics, photo chemistry, capture of solar energy and molecular design of devices. The Center for Exploitation of Solar Energy, Department of Chemistry, University of Copenhagen

2014: 10th *Congress* of the World Association of Theoretical and *Computational Chemists* WATOC 2014, Santiago Chile.

2014: 8th International Meeting on Photodynamics, Oaxaca, Mexico

2014: XL International Conference of Theoretical Chemists of Latin Expression, Quitel, Galapago Islands, Ecuador

2015: The Batsheva de Rothschild Seminar on Molecular Electronics 2015. 40 Years Later, Jerusalem, Israel

2015: International Workshop on: Charge, Heat and Energy Transport in Molecular Junctions.

2015: Chirality at the Nanoscale, Leuven, Belgium

2015: XVIII Symposium Brazilian Society of Theoretical Chemistry (SBQT)

2015: Pacifichem, Honolulu, Hawaii

2016: Telluride Science Research Center Workshop “Electronic and Magnetic Properties of Chiral Structures and their Assemblies”, June 27-July 01, Telluride, CO, USA.

Conferences by requested participation

1980: International Summer Institute in Quantum Chemistry and Solid State Physics, Loppi, Finland and Uppsala, Sweden.

1981: Nordic Molecular Physics Symposium, Ulvik, Norway.

1982: IVth International Congress in Quantum Chemistry, Uppsala, Sweden.

Curriculum Vitae Vladimiro Mujica

1982: Nordic Research Institute: Spectroscopic Methods in Surface Science, Gothenburg, Sweden.

1983: National Meeting in Atomic and Molecular Physics, Stockholm, Sweden.

1983: Xth International IUPAC Conference on Few Body Problems in Physics, Karlsruhe, Germany.

1983: XIIth International Colloquium on Group Theoretical Methods in Physics, Trieste, Italy.

1983: IIIth International Conference on Recent Progress in Many Body Theories, Odenthal-Altenberg, Germany.

1984: Nordic Molecular Physics Symposium, Svenborg, Denmark.

1984: Advanced Summer Institute in Electronic Structure of New Materials, Kuggom, Finland.

1985: National Meeting in Atomic and Molecular Physics, Lund, Sweden.

1985: Nordic Molecular Physics Symposium, Tallberg, Sweden.

1985: NATO Advanced Study Institute: Advances in Chemical Reaction Dynamics, Iraklion, Greece.

1986: Sanibel Symposium in Quantum Chemistry and Solid State Physics, MarineLand, Florida, U.S.A.

1986: 1st LatinAmerican -Florida Workshop on Quantum Sciences, Gainesville, Florida, U.S.A

1986: 1st national Meeting in Photochemistry, Uppsala, Sweden.

1986: Congreso Ibero-Americano de Catálisis, Mérida, Venezuela.

1987: Conference on Statistical Mechanics of Surfaces, Membranes and Polymers, Jerusalem, Israel.

1988: VIth International Congress in Quantum Chemistry, Jerusalem, Israel.

1988: Satellite Meeting on Chemical Reaction Dynamics, Rehovot, Israel.

1988: Symposium on Dynamical Processes in Condensed Molecular Systems, Jerusalem, Israel.

1989: Sanibel Symposium in Quantum Chemistry and Solid State Physics, St. Augustine, Florida, U.S.A

1989: 3rd LatinAmerican -Florida Workshop on Quantum Sciences, Gainesville, Florida, U.S.A

1990: Escuela Latinoamericana de Física, IVIC, Caracas, Venezuela.

1990: XIX Congreso Internacional de Químicos Teóricos de Expresión Latina, Rome, Italy.

1990: Workshop on Random Processes, University of West Indies, Barbados.

Curriculum Vitae Vladimiro Mujica

1991: Advanced NATO Study Institute. "Methods in Computational Molecular Physics". Bad Windsheim, Germany.

1992: XX Congreso de Químicos Teóricos de Expresión Latina. Mérida Venezuela.

1993: XXVI Midwest Theoretical Chemistry Conference. Carbondale, Illinois, U.S.A.

1993: Sanibel Symposium in Quantum Chemistry and Solid State Physics, St. Augustine, Florida, U.S.A.

1993: American Chemical Society Meeting, Chicago, Illinois, U.S.A

1993: XXI Congreso de Químicos Teóricos de Expresión Latina. Grenoble France.

1994: Encuentro de la Asociación Venezolana para el Avance de la Ciencia. Coro, Venezuela.

1994: II Congreso Venezolano de Química. Puerto La Cruz, Venezuela.

1995: XXI Congreso de Químicos Teóricos de Expresión Latina, Pucón, Chile.

1996: XLVI Convención Anual de AsoVAC. Barquisimeto, Venezuela.

1997: XLVII Convención Anual de AsoVAC. Valencia, Venezuela.

1997: I Congreso Venezolano de Física, Mérida, Venezuela,

AWARDS AND FELLOWSHIPS

FONINVES, Venezuela
Undergraduate studies fellowship
1977-1979.

FONINVES-CEPET
Graduate studies fellowship
1980-1986.

Researcher Level I. National System for Researchers Promotion,
Venezuela.
1990-1992.

Researcher Level II. National System for Researchers Promotion,
Venezuela.
1993-1999.

Premio Conicit al Mejor Trabajo Científico del Año 1998 en el Area de Química por el trabajo (National Research Council Prize To The Best Annual Scientific Work In Chemistry):
"Applications of photothermal displacement spectroscopy to the study of asphaltenes adsorption"
Optics Communications 145,(1997)69-75.

Researcher Level III. National System for Researchers Promotion Venezuela. 2000-2002.

Researcher Level IV (Highest level). National System for Researchers Promotion Venezuela. 2000-2002.

Researcher Level IV (Highest level). National System for Researchers Promotion Venezuela. 2007-2012.

Premio Conicit al Mejor Trabajo Científico del Año 2000 en el Area de Química por el trabajo (National Research Council Prize To The Best Annual Scientific Work In Chemistry):
"Caging of Molecules by Asphaltenes. A Model for Free Radical Preservation In Crude Oils Based on Intermolecular Energies of PAH"
Energy and Fuel 14(2000)632.

Lorenzo Mendoza Fleury Prize "Fundación Polar" for Science, Venezuela 2001.

Jose Maria Vargas Medal. First Class. Universidad Central de Venezuela, 2005.

International Workshop on Charge, Heat and Energy Transport in Molecular Junctions. An international symposium organized on the occasion of my birthday to celebrate my scientific career. University of Copenhagen, 2015

MEMBERSHIP IN SCIENTIFIC SOCIETIES

- Sociedad Venezolana de Física
- Sociedad Venezolana de Química.
- New York Academy of Sciences.
- American Physical Society
- American Chemical Society
- American Association for the Advancement of Science
- Asociación para el Progreso de la Investigación Universitaria de la U.C.V.
- Asociación Venezolana para el Avance de la Ciencia.

- Coordinator for Venezuela of the Florida-LatinAmerica Exchange Program in Quantum Sciences.

ADVISORY TO GRADUATE THESIS AND UNDERGRADUATE SPECIAL RESEARCH WORK

Doctoral Thesis:

- (1) Manuel Caetano, Universidad Central de Venezuela. Octubre (1993). "Estudios básicos y aplicados de plasmas a presión atmosférica inducidos por radiación de microondas". (Basic and applied studies of microwave induced plasmas at atmospheric pressure).
- (2) Emilio Squitieri. Universidad Central de Venezuela (1994). "Susceptibilidades ópticas para una molécula de dos niveles con acoplamiento intra-molecular y momento dipolar permanente no-nulo". (Optical susceptibilities of a two-level molecule with non vanishing permanent dipole moment and intramolecular coupling).
- (3) Ramiro Pino. Instituto Venezolano de Investigaciones Científicas (1997). "Potenciales y funcionales en la teoría del funcional de la densidad". (Functionals and Potentials in Density Functional Theory)
- (4) Inés Urdaneta. Universidad Central de Venezuela. Université de Paris Sud-Orsay (2006). "Laser-assisted Electron Transport in Nano-junctions: Theoretical Modelling" .
- (5) Luis Puerta. Universidad Central de Venezuela. (2009) "Estudio del Proceso de Transferencia de Carga Dipolo-Superficie en Función del Empaquetamiento en Películas Orgánicas Delgadas".
- (6) José Guaregua. Universidad Central de Venezuela (2008) "Difusión de Partículas Coloidales Esféricas Interactuando con un Potencial DLVO".
- (7) Dalvin Méndez, Arizona State University. Thesis work in progress.
- (8) Reza Vatan, Arizona State University, Thesis work in progress.
- (9) Angelo Di Bernardo, Arizona State University, Thesis work in progress.
- (10) Marely Tejada, Arizona State University, Thesis work in progress
- (11) Luis González, Arizona State University, Thesis work in progress.
- (12) Shobeir Khezerseddigh, Arizona State University, Thesis work in progress.
- (13) Micah Wimmer, Arizona State University, Thesis work in progress.

Co-supervisor of Postdoctoral Fellows in the Chemistry Department of Northwestern University:

- (1) Mathieu Kemp.
- (2) Adrian Roitberg

Co-supervisor of graduate students in the Chemistry Department of Northwestern University:

- (1) Yi Mao.

(2) Yaping Xu.

Undergraduate Special Research Work

- (1) Manuel Malaver, Escuela de Química, Facultad de Ciencias, Universidad Central de Venezuela, Marzo (1993).
"Estudio teórico del mecanismo de conducción iónica en poli-óxido de etileno".
(Theoretical Study of the Mechanism for Ionic Conduction in poly(ethylene oxide)).
- (2) BSc of Amanda Cheong. Goshen College, Goshen Indiana (1995).
"Effective Electronic Coupling in Intramolecular non-adiabatic electron transfer reactions".
- (3) Manuel Rojas, Escuela de Química, Facultad de Ciencias, Universidad Central de Venezuela (1996).
"Estudio crítico de la cuasi-degeneración electrónica y su influencia en la evaluación de energía y la geometría, con métodos semiempíricos. Caso MINDO/SR-UHF".
(A critical study of electronic quasi-degeneration and its influence in energy evaluation and geometry optimization using semi-empirical methods).
- (4) Alejandro Acevedo, Escuela de Química, Facultad de Ciencias, Universidad Central de Venezuela (1996).
"Influencia del movimiento nuclear en las particiones viriales regionales de una molécula diatómica".
(Influence of nuclear motion on the regional virial partitions of a diatomic molecule).
- (5) Natalia León. Escuela de Química, Facultad de Ciencias, Universidad Central de Venezuela (1998).
"Tiempos de residencia electrónicos en alambres moleculares".
(Electronic residence times in molecular wires).
- (6) Luis Puerta. Escuela de Química, Facultad de Ciencias, Universidad Central de Venezuela (1998).
"Estudio de estabilidad de agregados de asfaltenos mediante química computacional".
(Computational Chemistry Studies of Stability of Asphaltene Aggregates).
- (7) Eduardo Román. Escuela de Química, Facultad de Ciencias, Universidad Central de Venezuela (1999).
"Aplicación del modelo de spin de Heisenberg al problema de conducción electrónica en alambres moleculares"
(A Heisenberg spin model of electronic conduction in molecular wires).
- (8) Aileen Loszán. Escuela de Química, Facultad de Ciencias, Universidad Central de Venezuela (1999).
"Un estudio ab initio mecánico cuántico de la estabilidad de fragmentos asfálticos".
(An ab initio quantum mechanical study of the stability of asphaltenic fragments).
- (9) María Gorayeb. Escuela de Química, Facultad de Ciencias, Universidad Central de Venezuela (2002).
Un modelo para propiedades ópticas no lineales de moléculas push-pull.
(A model for nonlinear optical properties of push-pull molecules)
- (10) Gladys León, Escuela de Física, Universidad Central de Venezuela (2003)
Un modelo correlacionado para transporte de dos electrones en gotas cuánticas"
(A correlated model for two-electron transport in quantum dots)
- (11) Raiza Hernández, Escuela de Química, Universidad Central de Venezuela (2004)
Estudio atomístico del proceso de ruptura de alambres metálicos.
(An atomistic study of the breaking process of atomic wires)
- (12) Luis Montano, Arizona State University, work in progress.

Co-supervisor of Minority Student in the Summer Research Opportunities Program at Northwestern University:

- (1) Thaddeus Jones, Jackson State University

RESEARCH PROJECTS

- (1) "Transporte de carga en polímeros electroactivos y electrolitos iónicos".
(Charge transport in electroactive polymers and ionic electrolites).

Funding: C.D.C.H-U.C.V

Participation: Principal Investigator.

Status: Concluded.

- (2) "Estudio teórico-experimental de la respuesta termo-óptica de soluciones".
(Experimental theoretical study of the thermo-optical response of solutions).

Funding: C.D.C.H-U.C.V and CONICIT.

Participation: Principal Investigator.

Status: Concluded.

- (3) "Theoretical and Computational Developments in Density Functional Theory of Many-Electron Systems: Adiabatic and Non-Born-Oppenheimer N-representable Local-Scaling Version of Density Functional Theory and its Coupling with the Colle-Salvetti Ansatz"

Funding: Economic European Community.

Participation: Associate Investigator .

Status: Concluded.

- (4) Estudio de la respuesta termoóptica de sistemas químicos complejos.
(Study of the thermo-optical response of complex chemical systems).

Funding: CONICIT.

Participation: Principal Investigator.

Status: Concluded.

- (5) Conduction in mesoscopic devices.

Funding: CONICIT-National Science Foundation (U.S.A.).

Participation: Principal Investigator, Venezuelan counterpart.

Status: Concluded.

- (6) Electronic Transport in Hybrid Materials

Funding: CONICIT-National Science Foundation (U.S.A.).

Participation: Principal Investigator, Venezuelan counterpart.

Status: Concluded.

- (7) Fuerzas intermoleculares y la teoría del funcional de densidad.
(Intermolecular forces and density functional theory)

Funding: CONICIT.

Participation: Associated Investigator.

Status: Concluded.

- (8) Fisicoquímica de sistemas dispersos.
(Physical Chemistry of Disperse Systems)

Funding: CONICIT.

Participation: Associated Investigator.

Status: Concluded.

Curriculum Vitae Vladimiro Mujica

(9) Molecular Nanoelectronics: Simulation from Molecules to Circuits.

Funding: NSF

Participation: International Advisor and Associate Investigator.

Status: Concluded.

(10) Research Award Argonne National Laboratory

Funding: Argonne National Laboratory

Participation: Principal Investigator

Status: 2005-2009

(11) Start-up Grant, Arizona State University, MP11004 \$200,000.00

Status: Active

(12) NSF 1124895 International Collaboration in Chemistry: A Theoretical Investigation Of The Role Of The Chemical Bond In The Raman And Fluorescence Response Of Molecule-Nanoparticle Hybrids CHE COLLABORATIVE RESEARCH, Theory, Models, Comput. Method \$400,000.00

Participation: PI

Status: Active

(13) NSF-ENG-CBET 1236571 Transport-Enhanced Thermogalvanic Energy Conversion. Start date-End date 9/15/2012-8/31/2017. \$300,000.00

Participation: PI

Status: active

(14) DE-AR0000343 DOE-ARPA Energy Efficient Electrochemical Capture and Release of Carbon Dioxide. 3/12/2013-3/11/2014. \$662,130.00

Participation: Co-PI

Status: Active

February 12, 2017