CURRICULUM VITÆ

RECENT RESEARCH ACHIEVEMENTS, ACTIVITIES AND SHORT CURRICULUM VITAE OF

PROF. RODOLFO O. ESQUIVEL OLEA

1. **Recent research achievements**

2. **Short Curriculum Vitae**

1. RECENT RESEARCH ACHIEVEMENTS

World leader in Applications of Information Theory in Chemistry and Nanostructured Materials

Information Theory (IT) concepts are at the borderline of the development of the physical sciences which are attracting the attention of numerous researchers. In the present review article we discuss several applications of IT to the study of chemical systems and processes. This area of inquiry is shedding new light on the conceptual foundations of quantum chemistry and physics and is also at the core of the new field of quantum information theory, which foresees important technological developments through concepts such as "entanglement", "teleportation" and "quantum computation". Besides, there is an inherent interest for applying the new entropic and complexity ideas and methodologies to chemical and biological systems and their processes. In line with these developments we have undertaken multidisciplinary research projects so as to employ IT at different levels, classical (Shannon, Fisher, complexity, etc) and quantum (von Neumann and other entanglement measures) on a variety of chemical processes, organic and nanostructured molecules. Recently, significant advances in chemistry have been achieved by use of Shannon entropies through the localized/delocalized features of the electron distributions allowing a phenomenological description of the course of elementary chemical reactions by revealing important chemical regions that are not present in the energy profile such as the ones in which bond forming and bond breaking occur. Further, the synchronous reaction mechanism of a S_N2 type chemical reaction and the non-synchronous mechanistic behavior of the simplest hydrogenic abstraction reaction were predicted by use of Shannon entropies analysis. In addition, a recent study on the three-center insertion reaction of silylene has shown that the information-theoretical measures provide evidence to support the concept of a continuum of transient of Zewail and Polanyi for the transition state rather than a single state, which is also in agreement with other analyses. While the Shannon entropy has remained the major tool in IT, there have been numerous applications of Fisher information through the "narrowness/disorder" features of electron densities in conjugated spaces. Thus, in chemical reactions the Fisher measure has been employed to analyze its local features and also to study the steric effect of the conformational barrier of ethane. Complexity of the physical, chemical and biological systems is a topic of great contemporary interest. The quantification of complexity of real systems is a formidable task, although various single and composite information-theoretic measures have been proposed. For instance, Shannon entropy (S) and the Fisher information measure (I) of the probability distributions are becoming increasingly important tools of scientific analysis in a variety of disciplines. Overall, these studies suggest that both S and I can be used as complementary tools to describe the information behavior, pattern, or complexity of physical and chemical systems and the electronic processes involving them. Besides, the disequilibrium (D), defined as the expectation value of the probability density is yet another complementary tool to study complexity since it measures its departure from equiprobability. Thus, measuring the complexity of atoms and molecules represents an interesting area of contemporary research which has roots in information theory. In particular, complexity measures defined as products of S and D or S and I have proven useful to analyze complexity features such as order, uncertainty and pattern of molecular systems and chemical processes. On the other hand, the most interesting technological implications of quantum mechanics are based on the notion of entanglement, which is the essential ingredient for the technological implementations that are foreseen in the XXI century. Up to now it remains an open question whether entanglement can be realized with molecules or not and hence it is evident that the new quantum techniques enter the sphere of chemical interest. Generally speaking, entanglement shows up in cases where a former unit dissociates into simpler sub-systems, the corresponding processes are known quite well in chemistry. Although information entropies have been employed in quantum chemistry, applications of entanglement measures in chemical systems are very scarce. Recently, von Neumann measures in Hilbert space have been proposed and applied to small chemical systems, showing than entanglement can be realized in molecules. For nanostructures, we have been able to show that IT measures can be successfully employed to analyse the growing behaviour of PAMAM dendrimers supporting the dense-core model against the hollow-core one.

2. CURRICULUM VITAE

PERSONAL DATA

Family Name:	ESQUIVEL OLEA
First Name:	RODOLFO OCTAVIO
Born: Mexico City, México	05/08/1959
Family Status:	Four Children
Present Position:	Full Professor in Chemistry
Academic Institution:	Departamento de Química Universidad Autónoma Metropolitana Unidad Iztapalapa Av San Rafael Atlixco 186, Col. Vicentina
Phone:	+52 5558044967 (office)
Fax:	+52 5558044666
E-mail:	esquivel@xanum.uam.mx

EDUCATION

Degree	Institution	Date
B.Sc.	Metropolitan Autonomous University	1983
M.Sc..	Metropolitan Autonomous University	1985
Ph.D.	Metropolitan Autonomous University	1988

ACADEMIC EXPERIENCE

Position	Institution	Date
Assistant Professor	Metropolitan Autonomous University (Mex)	1983-1984
Associate Professor	Metropolitan Autonomous University (Mex)	1985-1989
Lecturer	Centre for Research and Advanced Studies at IPN (Mex)	1988-1990
Full Professor	Metropolitan Autonomous University (Mex)	1982 to date
Visiting Professor	Dept. of Physics, Queens University (Can)	1991-1992
Visiting Professor	Dept. of Physics, Queens University (Can)	1992-1993
Visiting Professor	Instituto Carlos I de Física Teórica (Spain)	2008-2009
Visiting Professor	Instituto Carlos I de Física Teórica (Spain)	2010
Visiting Professor	Instituto Carlos I de Física Teórica (Spain)	2012

PROFESSIONAL SOCIETIES

Society	Membership
Mexican Chemical Society	1984 -
Mexican Physical Society	1989 -
Society for Theoretical Chemical Physics	1992 -
Mexican Academy of Sciences	1997 -
American Chemical Society	2007 -

AWARDS

Weizmann Prize in Physical Sciences (granted by the Weizmann Institute, Israel)	1989
Diploma for scientific achievements (granted by UAM)	1990
Biography in "*Who is Who in the World*", Ed. 1999	1999
Queen's Research Award granted (granted by the advisory research committee at Queen's University, Canada)	1992
Fellow of the National Science Programme (Funded by the Ministry of Science and Technology, Mexico):	
- Candidate	1985-1990
- Fellow (Level I)	1991-1994
- Fellow (Level II)	1997 to date
- Fellow (Level III)	2012 to 2016

* UAM: Metropolitan Autonomous University

ACADEMIC MANAGMENT ACTIVITIES

Elected secretary for the evaluating committee of the academic personnel of CBI at UAM	1989-1990
Member of the organizing committee of the symposium for graduate science studies: Fernando Romo	1986-1989

Member of the Supercomputer Centre Committee at UAM	1993-1999
Chairman of the BSc graduate studies in Chemical Sciences at UAM	1994-1999
Chairman of the PhD graduate studies in Chemical Sciences at UAM	1999-2004
Codesigner of the Graduate Studies program at CBI, UAM	
Member of the Graduate Studies Committee at UAM	1994-2004
Member of the evaluating committee for the academic personnel of the Faculty of Chemistry and Biological Sciences at FES-Zaragoza, UNAM	2005-2008
Codesigner of the major plan for the B.Sc. studies in chemistry at UAM	2007-2008

* CBI: Division of Basic Sciences and Engineering
* UAM: Metropolitan Autonomous University
* UNAM: National Autonomous University of Mexico

PH. D. ADVISEES

Advisee	Graduation
Juan Carlos Ramírez García Dissertation subject: "Some Applications of Information Theory in Chemistry".	2001
Catalina Soriano Correa Dissertation subject: "Theoretical study of the structure-activity relation of anti-lepra compounds"	2003
Nicolaís Guevara León Dissertation subject: "Estudio de las entropías informacionales en Sistemas atómicos y moleculares"	2003
Nelson Flores Gallegos Dissertation subject: "Quantum Information Theory: A conceptual language for Chemistry"	2010
Edmundo Carrera Martínez Dissertation subject: "Chemical Reactivity and Quantum Information Theory"	In process
Gabriel Molina Espíritu	In process

M.Sc. ADVISEES

Advisee	Graduation

Ana Lilia Rodríguez Sánchez 1995
Dissertation subject: "Theoretical study of the variational effects on the electron atomic densities".

Juan Carlos Ramírez García. 1995
Dissertation subject: "Theoretical study of organometallic manganesic compounds and accurate determination of IR frequencies of ethanes and deuterated species"

Catalina Soriano Correa. 1997
Dissertation subject: "Theoretical study of anti-Lepra agents"

Elizabeth Escamilla Roa. 2000
Dissertation subject: "Theoretical study of selected chemical reactions of environmental chemistry: Information theory"

Juan Francisco Sánchez Ruiz. 2006
Dissertation subject: "Estudio farmacológico de antibióticos β-Lactámicos mediante parámetros mecánico-cuánticos"

TEACHING EXPERIENCE

Undergraduate level:

General Chemistry, Chemicals Physics, Quantum Chemistry, Atomic and Molecular Structure, Thermodinamics, Computational Chemistry.

Graduate level:

Quantum Chemistry, Atomic and Molecular Structure, Computational Physical Chemistry, Advanced Topics in Quantum Chemistry, Group Theory

PEER REVIEW EXPERIENCE

Physical Review Letters

Physical Review A

Physical Review B

Journal of Molecular Structure: THEOCHEM

Grants committee, CONACyT (National Science Foundation)

Journal of the Mexican Chemical Society

European Journal of Medicinal Chemistry

Journal of Molecular Graphics and Modelling

Journal of Information Sciences

International Journal of Applied Mathematics and Statistics

Sof t Matter

RESEARCH INTERESTS

Physics: atomic and molecular structure, Shannon information theory, quantum information theory, statistical complexity, nanostructures materials

Chemistry: molecular properties, chemicals reactions, dissociation processes, conformational analysis, stereochemistry, supramolecular systems, weak interactions

Biology: physicochemical properties of biological systems, theoretical pharmacology, molecular similarity

RESEARCH GRANTS

Name	Sponsor	Reference	Period
Constrained atomic electron densities	CONACyT	1799-E9210	1993-1994
Theoretic information study of Atoms: effect of correlation	CONACyT	4970-E9406	1995-1996
Physicochemical properties of Anti-lepra compunds	CONACyT	29286-E	1998-2002
Theoretic information study of chemical reactions	CONACyT	2007-82266	2008-2009
Sabbatical leave	CONACyT	80604	2008
Research award	Ministerio de Educación, España		2010
Information and complexity Measures	CONACyT	2011-80244	2011-2014

SUPERCOMPUTING EXPERIENCE

Name	Location	Period
Cray, Berenice , Kan Balam	UNAM	1993-2011
CDC, Titan, Snakes, SGI, CM5, IBM-RS6000, Aitzaloa	UAM-Iztapalapa	1991-2011
SP2-IBM	Cornell Supercomputing Center	1991
IBM-RS6000	Queens University	1991-1992
UGR-Grid (1300 CPU)	Universidad de Granada	2009-2011
MareNostrum (10240 CPU)	Universidad de Barcelona	2010

CONFERENCE ATTENDANCE

5th International Congress on Quantum Chemistry. University of Montreal, Montreal, Quebec, Canada	1985
Satellite Symposium on Molecular Structure and Chemical Reactivity. University of Toronto, Canada	1985
6th Latin American Workshop on Theoretical Chemistry Centro de Pesquisas Fisicas, Rio de Janeiro, Brasil	1988
10th Canadian Symposium on Theoretical Chemistry University of Calgary, Banff, Alberta, Canada	1989
Queen's Materials Research Conference Queen's University-Alcan Canada, Kingston, Canada	1991
First Canadian Symposium on Computational Chemistry Université de Sherbrooke, Quebec, Canada	1991
Electronic Structure '91 Cornell Theory Center, Cornell University, New York, USA	1991
IBM-AIX/370 Supercomputer Workshop Cornell National Supercomputer Facility, New York, USA	1991
NSERC-CAP Summer Institute in Theoretical Physics: DFT: Methods and Applications, Queen's University, Canada	1992
11th Canadian Symposium on Theoretical Chemistry Mc-Gill University-Université de Montréal, Quebec, Canada	1992
Nato Advanced Study Institute: Relativistic and Correlation Effects University of British Columbia, Vancouver, Canada	1992
Density Functional Theory and its Applications: A Conference in Honour to Prof. N. H. March, University of Oxford, UK	1992

First Congress of the International Society for Theoretical Chemical Physics Universitat de Girona , Girona, Catalunya, España	1993
2nd Canadian Symposium on Computational Chemistry Queen's University, Kingston, Ontario, Canada	1994
Thirty Years of Density Functional Theory Jagiellonian University, Cracovia, Polonia	1994
8th International Congress on Quantum Chemistry. Academy of Sciences of the Czech Republic, Praga, Republica Checa	1994
12th Canadian Symposium on Theoretical Chemistry University of New Brunswick, Fredericton, Canada	1995
36th Sanibel Symposium University of Florida, St. Augustine, Florida, USA	1996
1996 American Conference on Theoretical Chemistry University of Utah, Park City, Utah, USA	1996
9th International Congress on Quantum Chemistry Atlanta, Georgia, USA	1997
VI Congreso Iberoamericano de Química Inorgánica Puebla, México	1997
XXIV Congreso Internacional de Químicos Teóricos de Expresión Latina, Puebla, México	1998
Third Congress of the International Society for Theoretical Chemical Physics, México, D.F.	1999
10^{th} Conference on Current Trends in Computational Chemistry Jackson, Mississippi, USA	2001
43 Sanibel Symposium, St. Augustine Florida, USA	2003
Quantum Systems in Chemistry and Physics Spetses-Hellas, Grecia	2003
44th Sanibel Symposium, St Augustine, Florida, USA	2004
XXXI Congreso de Químicos Teóricos de Expresión Latina Margarita, Venezuela	2005
III Internacional-XXXVIII Congreso Nacional de Ciencias Farmacéuticas Veracruz, Ver.	2005
ESPA 2006 Electronic Structure: Principles and Applications Santiago de Compostela, España	2006
6th Canadian Computatonal Chemistry Conference University of British Columbia, Canada	2006
12th edition of the International Conference on the Applications of DFT in Chemistry and Physics, Amsterdam, Holanda	2007

Special Functions, Information Theory and Mathematical Physics" 2007
An interdisciplinary conference in honor of Prof. JesÃºs S. Dehesa's 60th birthday.
Granada, España

2008 NSTI Nanotechnology Conference and Trade Showing Generation 2008
Boston, Massachussetts

PAMAM Dendrimers of Goewing Generation, 3rd Mexican Workshop 2008
on Nanostructured Materials, CInvestav, México

International Dendrimer Symposium 6 2009
Stockholm Sweden

14th International Workshop On Quantum Systems In Chemistry And Physics 2009
San Lorenzo de El Escorial, Madnd (Spain)

XXXV Congress of Theoretical Chemists of Latin 2009
San Andrés, Colombia

10th European Conference on Atoms, Molecules and Photons 2010
Salamanca, Spain

15th International Workshop On Quantum Systems In Chemistry And Physics 2010
Cambridge, England

Jensen–Tsallis divergence and atomic dissimilarites for neutral and ionized 2010
systems in conjugated spaces"
J.C. Angulo, J. Antolin, S. López-Rosa, R.O. Esquivel

10th EUROPEAN CONFERENCE ON ATOMS, MOLECULES AND PHOTONS
Julio 5-9, 2010
Salamanca, España

"Entropic study of the transition state, and the bond breaking and bond 2010
forming processes of selected elementary chemical reactions in conjugated spaces"
R. O. Esquivel, N. Flores-Gallegos, Cristina Iuga, Edmundo M. Carrera, J. C. Angulo, J. Antolin
15TH INTERNATIONAL WORKSHOP ON QUANTUM SYSTEMS IN CHEMISTRY AND PHYSICS
September 1-5 (2010)
Cambridge, England

"Hacia la Nueva Ciencia de la Química de Información" 2011
Rodolfo O. Esquivel, Juan Carlos Angulo, Juan Antolín, Jesús S. Dehesa,
R. Plastino, Edmundo Martínez Carrera, Nelson Flores-Gallegos,
Moyocoyani Molina-Espíritu, Cristina Iuga,
IV Reunión de la División de Información Cuántica (IV DICU)
Centro Nacional de Metrología, CENAM,
28 al 30 de abril, 2011

"Quantum Entanglement and the Dissociation Process of Diatomic Molecules" 2011
Rodolfo O. Esquivel, Nelson Flores-Gallegos, Moyocoyani Molina-Espíritu,
A. R. Plastino, Juan Carlos Angulo,Juan Antolín and Jesús S. Dehesa
IV Reunión de la División de Información Cuántica (IV DICU)
Centro Nacional de Metrología, CENAM,

28 al 30 de abril, 2011

"La entropía y el problema de la inseparabilidad en sistemas cuánticos moleculares" 2011
Edmundo Carrera and Rodolfo O. Esquivel
IV Reunión de la División de Información Cuántica (IV DICU)
Centro Nacional de Metrología, CENAM,
28 al 30 de abril, 2011

"Hacia la Nueva Ciencia de la Química de Información" 2011
Química Teórica en el Siglo XXI
Facultad de Química, UNAM
19 a- 21 de Sept. 2011

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1 NOMBRE DEL EVENTO 10th EUROPEAN CONFERENCE ON ATOMS, MOLECULES AND PHOTONS
LUGAR: Salamanca, España
NOMBRE DEL TRABAJO "Jensen-Tsallis divergence and atomic dissimilarites for neutral and ionized systems in conjugated spaces"
FECHA: Julio 5-9, 2010

2 NOMBRE DEL EVENTO 15TH INTERNATIONAL WORKSHOP ON QUANTUM SYSTEMS IN CHEMISTRY AND PHYSICS
LUGAR: Cambridge, England
NOMBRE DEL TRABAJO "Entropic study of the transition state, and the bond breaking and bond forming processes of selected elementary chemical reactions in conjugated spaces"
FECHA: September 1-5 (2010)

3 NOMBRE DEL EVENTO: III Jornadas de Investigadores de FIsica en Atómica y Molecular.
LUGAR: Madrid, España
NOMBRE DEL TRABAJO: Complexity measures and information planes of molecular densities.
FECHA: 2011/02/03.

4 NOMBRE DEL EVENTO: IV Reunión de la División de Información Cuántica (IV DICU).
LUGAR: Queretaro, México
NOMBRE DEL TRABAJO: Hacia la Nueva Ciencia de la Química de Información.
FECHA: 2011/04/28.

5 NOMBRE DEL EVENTO: IV Reunión de la División de Información Cuántica (IV DICU).
LUGAR: Queretaro, México
NOMBRE DEL TRABAJO: La entropía y el problema de la inseparabilidad en sistemas cuánticos moleculares.
FECHA: 2011/04/28.

6 NOMBRE DEL EVENTO: IV Reunión de la División de Información Cuántica (IV DICU).
LUGAR: Queretaro, México

NOMBRE DEL TRABAJO: Quantum Entanglement and the Dissociation Process of Diatomic Molecules.
FECHA: 2011/04/28.

7 NOMBRE DEL EVENTO: THe Madrid Conference on Femtochemistry FEMTO10.
LUGAR: Madrid, España
NOMBRE DEL TRABAJO: Fisher Information Study for Elementary Chemical Reactions.
FECHA: 2011/07/10.

8 NOMBRE DEL EVENTO: QUANTUM MATTER.
LUGAR: Granada, Españ
NOMBRE DEL TRABAJO: Jensen-Tsallis Divergence and Dissimilarity for neutral and ionized systems.
FECHA: 2011/09/18.

9 NOMBRE DEL EVENTO: X Reunion Mexicana de Fisicoquímica Teórica.
LUGAR: Pachuca, México
NOMBRE DEL TRABAJO: Compleidad Estadistica en Reacciones Quimicas Elementales.
FECHA: 2011/11/10.

10 NOMBRE DEL EVENTO: X REUNIÓN MEXICANA DE FISICOQUÍMICA TEÓRICA.
LUGAR: Pachuca, México
NOMBRE DEL TRABAJO: Estudio computacional de la influencia de grupos electrodonadores y electroatractores en la estructura electronica de un peptido.
FECHA: 2011/11/10.

CONFERENCIAS INVITADAS (4)

1 NOMBRE DEL EVENTO: CIclo de Seminarios del Departamento de QUimica, UAMI.
LUGAR: UAM, México
CONFERENCIA: Hacia la Nueva Ciencia de la QUimica de Información.
FECHA: 2011/03/23.

2 NOMBRE DEL EVENTO: IV Reunion de la DIvision de Informacion CUantica.
LUGAR: Queretaro, México
CONFERENCIA: Hacia la NUeva Ciencia de la Quimica de Informacion.
FECHA: 2011/04/28.

3 NOMBRE DEL EVENTO: QUIMICA TEORICA EN EL SIGLO XXI.
LUGAR: UNAM, México
CONFERENCIA: Hacia la Nueva CIencia de la QUimica de Informacion.
FECHA: 2011/09/18.

4 NOMBRE DEL EVENTO: FISyMAT UNIVERSIDAD DE GRANADA.

LUGAR: Granada, España
CONFERENCIA: Procesos Concurrentes en Reacciones Químicas.
FECHA: 2012/02/15.

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1. NOMBRE DEL EVENTO Iberian Meeting on Atomic and Molecular Physics (IBER2013).
   LUGAR: Sevilla, España
   NOMBRE DEL TRABAJO "Entanglement of selected elementary chemical reactions"
   FECHA: 10/09/2013.

2. NOMBRE DEL EVENTO Iberian Meeting on Atomic and Molecular Physics (IBER2013).
   LUGAR: Sevilla, España
   NOMBRE DEL TRABAJO "Quantum entanglement of He isoelectronic series"
   FECHA: 10/09/2013.

3. NOMBRE DEL EVENTO QUITEL2013
   LUGAR: Granada, España
   NOMBRE DEL TRABAJO "Quantum Information Chemistrv: Entanglement of Elementarv Chemical Reactions"
   FECHA: 30/06/2013.

NOMBRE DEL EVENTO VII Reunión Anual de la División de Información Cuántica de la Sociedad Mexicana de Física
LUGAR: Cuernavaca, México
NOMBRE DEL TRABAJO "Entanglement of selected elementary chemical reactions"
FECHA: 7-9/05/2014.

NOMBRE DEL EVENTO : 10th Congress of the World Association of Theoretical and Computational Chemists
LUGAR: Santiago, Chile
NOMBRE DEL TRABAJO "Quantum Information-Theoretical Aspects of Elementary Chemical Processes : Concurrent Processes and Entanglement"
FECHA: 5-10/10/2014.

NOMBRE DEL EVENTO: 10th Congress of the World Association of Theoretical and Computational Chemists
LUGAR: Santiago, Chile
NOMBRE DEL TRABAJO "Quantum Entanglement and the spooky action at distance "
FECHA: 5-10/10/2014.

NOMBRE DEL EVENTO 10th Congress of the World Association of Theoretical and Computational Chemists
LUGAR: Santiago, Chile
NOMBRE DEL TRABAJO "Information theoretical Analysis of Biological Molecules"
FECHA: 5-10/10/2014.

SCIENTIFIC PUBLICATIONS

ARTICLES

1. Simple correlated wave functions for accurate electron densities: An application to neon
A.V. Bunge and R.O. Esquivel,
Physical Review A 34, 853 (1986).

2. Accurate electron density and one-electron properties for Be
R.O. Esquivel and A.V. Bunge,
International Journal of Quantum Chemistry 32, 295 (1987).

3. Spin density and density moments for the lithium ground state
R.O. Esquivel, A.V. Bunge and M.A. Núñez,
Physical Review A 43, 3373 (1991).

4. Reaction of (η3-Pentadienyl) tricarbonylmanganese with secondary amines. Synthesis and characterization of (1- amino-η3- pentenyl) tricarbonylmanganese complexes and their phosphine or tetracarbonyl derivatives, N. Zúñiga-Villarreal, M.A. Paz-Sandoval, P. Joseph-Nathan and R.O. Esquivel
Organometallics 10, 2616 (1991).

5. Electron correlation study on momentum-space: Be series
A.N. Tripathi, R.P. Sagar, R.O. Esquivel and V.H. Smith, Jr.
Physical Review A 45, 4385 (1992).

6. Accurate one-electron momentum-space properties for the Li isoelectronic sequence
R.O. Esquivel, A.N. Tripathi, R.P. Sagar and V.H. Smith, Jr.,
Journal of Physics B 25, 2925 (1992).

7. Pseudoatoms of the electron density
K. Edgecombe, R.O. Esquivel, V.H. Smith Jr. and F. Müller-Plathe,
Journal of Chemical Physics 97, 2593 (1992).

8. Pseudo-convexity of the atomic charge density: Lower and upper bounds
R.O. Esquivel, J. Chen, M.J. Stott, R.P. Sagar and V.H. Smith, Jr.
Physical Review A 47, 936 (1993).

9. Pseudo-convexity of the atomic charge density: A numerical study
R.O. Esquivel, R.P. Sagar, V.H. Smith, Jr., J. Chen, and M.J. Stott
Physical Review A 47, 4735 (1993).

10. Non-monotonicity of the atomic electron momentum density.
R.P. Sagar, R.O. Esquivel, H. Schmider, A.N. Tripathi, and V.H. Smith, Jr.
Physical Review A 47, 2625 (1993).

11. Spin Magnetic form factors in position and momentum space.
H. Schmider, R.O. Esquivel, R.P. Sagar, and V.H. Smith, Jr.
Journal of Physics B 26, 2943 (1993).

12. Atomic information entropies beyond the Hartree-Fock limit.
Minhhuy Hồ , R.P. Sagar, R.O. Esquivel, and V.H. Smith, Jr.
Journal of Physics B 27, 5149 (1994).

13. Exchange correlation potential for small atoms
J. Chen, R.O. Esquivel and M.J. Stott
Philosophical Magazine B 69, 1001 (1994).

14. A numerical study of molecular information entropies.
Minhhuy Hồ , R.P. Sagar, José M. Pérez-Jordá, V.H. Smith, Jr., and R.O. Esquivel
Chemical Physics Letters 219, 15 (1994)

15. Accurate elastic and inelastic scattering factors for He-Ne.
J. Wang, R.O. Esquivel, V.H. Smith, and C.F. Bunge,
Physical Review A 51, 3812 (1995)

16. Theoretical Chemistry in Latin America and the Caribbean.
R.O. Esquivel and E. Juarisiti
Science in Latin America and the Caribbean and its Role in Regional Development I, 316 (1995)

17. Electron correlation in momentum-space: Ne series
A.N. Tripathi, V.H. Smith, Jr., R.P. Sagar, and R.O. Esquivel
Physical Review A 54, 1877 (1996).

18. Physical interpretation of information theory: Numerical evidence of Collins' conjecture.
R.O. Esquivel, A.L. Rodríguez, R.P. Sagar, Minhhuy Hˆo, and V.H. Smith, Jr.
Physical Review A 54, 259 (1996)

19. Kohn-Sham efective potentials for spin polarized atomic systems.
J. Chen, J.B. Krieger, R.O. Esquivel, M.J. Stott and G.J. Iafrate
Physical Review A 54, 1910 (1996)

20. Jaynes Information Entropy of Small Molecules: Numerical evidence of Collins' conjecture.
J.C. Ramirez. C. Soriano, R.O. Esquivel, M. Ho, R.P. Sagar, and V.H. Smith

Phys Rev A 56, 4477 (1997)

21. Ab Initio Calculations for Some Photocromatic Alkalline Crystals.
J. Capilla, R.O. Esquivel, and J.E. Sánchez
Physical Review B, sometido (1999)

22. Molecular Similarity Based on Information Entropies
Minhhuy Hồ , V.H. Smith, Jr., D. Weaver, C. Gatti, R.P. Sagar, and R.O. Esquivel
Journal of Chemical Physics 108, 5469 (1998)

23. Accurate Determination of the Fermi Contact Interaction in Atomic Lithium
R.O. Esquivel, Annik Vivier-Bunge, and V.H. Smith
Journal of Molecular Structure: THEOCHEM 433, 43 (1998).

24. Calculating the Logarithmic Mean Excitation Energy from the Shannon Information Entropy of the Charge Density.
Minhhuy Hồ , D. Weaver, V.H. Smith, Jr., R.P. Sagar, and R.O. Esquivel
Physical Review A 57, 4512 (1998)

25. Amount of information present in the one-particle density matrix and the charge density
J.C. Ramirez, J.M. Hernández-Pérez, R.P. Sagar, R.O. Esquivel, Minhhuy Hồ , and Vedene H. Smith, Jr.
Physical Review A 58, 3507 (1998)

26. An Information-Entropic study of correlated densities of the water molecule
M. Hồ , D. Weaver, V. H. Smith, R.P. Sagar, R.O. Esquivel, and S. Yamamoto.
Journal of Chemical Physics 109, 10620 (1998)

27. Shannon entropy of chemical changes: SN2 displacement reactions
M. Hồ , H. Schmider, R.P. Sagar, and R.O. Esquivel.
 International Journal of Quantum Chemistry 77, 376 (2000)

28. Shannon information entropies of molecules and functional groups in the self-consistent reaction field
M. Hồ , James Clark, V. H. Smith, Donald F. Weaver, Carlo Gatti, R.P. Sagar, R.O. Esquivel
Journal of Chemical Physics 112, 7572 (2000)

29. Shannon information and logarithmic mean excitation energies from cusp and asympotic constrained model densities
R.P. Sagar, J.C. Ramírez, R. Esquivel, M. Hồ , and V. H. Smith
Physical Review A 63, 022509 (2001)

30. Cálculos ab-initio de agentes anti-lepra comparando sus estructuras y propiedades fisicoquímicas con un conjunto de compuestos análogos Catalina Soriano, R.O. Esquivel y R.P. Sagar
Revista Mexicana de Física 46, 108 (2000)

31. Erratum: Pseudoconvexity of the atomic electron density: A numerical Study
R.O. Esquivel, R.P. Sagar, V.H. Smith, Jr., J. Chen, and M.J. Stott
Physical Review A 61, 019901 (1999)

32. Asymptotic behaviour of the ratio of gradient to electron density for atomic systems
M. Hô , V. H. Smith, R.P. Sagar, and R.O. Esquivel
Molecular Physics 99, 1727 (2001).

33. Relationships between Jaynes entropy of the one-particle density matrix and Shannon entropy of the electron densities
R.P. Sagar, R.O. Esquivel, J.C. Ramirez, M. Hô , and Vedene H. Smith, Jr. .
Journal of Chemical Physics 116, 9213 (2002)

34. Physicochemical and Structural Properties of Bacteriostatic Sulfonamides: Theoretical Study
Catalina Soriano, R.O. Esquivel y R.P. Sagar
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Dr. Rodolfo O. Esquivel Olea