

Spiros S. Skourtis

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<http://ucy.ac.cy/dir/en/component/comprofiler/userprofile/skourtis> , www.biophys.ucy.ac.cy/phdsp/

Date of birth 26 February 1966

Citizenship Greek

Marital Status Married, two children

Current Position *Associate Professor (Biophysics & Chemical Physics)
Department of Physics, University of Cyprus, Nicosia, Cyprus*

Other Positions (2012) *Visiting Associate Professor (Research Group of Molecular Electronics) June -Aug
Israel Institute of Advanced Studies
The Hebrew University of Jerusalem, Jerusalem, Israel*

Research Interests Modeling of charge and energy transport in biological and molecular systems (solution, molecular junction, single molecule settings)
Open quantum systems theory for molecular rate processes in condensed phase environments
Chemical and biological tunneling phenomena
Structure-function and dynamics-function relationships for proteins

Education *Ph.D. Theoretical Biophysics* 1991
University of California Berkeley, USA

Dissertation Title

Theoretical Issues in Biomolecular Dynamics.
 (Investigation of the primary charge separation in photosynthesis, and of the theory
 of nonadiabatic transitions in electron transfer)

B.G.S. Physics & Mathematics 1986
University of Miami, Coral Gables, Florida, USA

**Professional
 Experience**

Department of Physics
University of Cyprus, CYPRUS
 Associate Professor Oct. 06 - present
 Chairperson Feb. 08 - Feb. 10

Tenure was awarded based on the recommendation of an international
 tenure-review committee comprised of:

Prof. James M. Lisy	(Chairperson)	Univ. of Illinois at Urbana-Champaign, USA
Prof. Marilyn Gunner		City College of New York, USA
Prof. Peter Hanggi		Univ. of Augsburg, Germany
Prof. Volkhard Helms		Center for Bioinformatics, Saarland Univ., Germany
Prof. Joel L. Sussman		Weizmann Institute of Science, Israel

Department of Physics Feb. 00 - Oct. 06
University of Cyprus, CYPRUS
 Assistant Professor

Department of Natural Sciences Jan. 97 - Feb. 00
University of Cyprus, CYPRUS
 Assistant Professor

Department of Chemistry Jan. 95 - Jan. 97
University of Pittsburgh, PA, USA
 Research Assistant Professor (96-97)
 Research Associate (95-96)
 Biophysics and Chemical Physics

Department of Chemistry Jan. 94 - Jan. 95
University of Rochester, NY, USA
 Postdoctoral Fellow
 Chemical Physics

Department of Physics Sept. 91 - Dec. 93
University of California San Diego, CA, USA
 Postgraduate Research Physicist

Biophysics and Chemical Physics

Lawrence Berkeley Laboratory May 90 - Aug. 90
Molecular and Chemical Sciences Division
University of California, CA, USA
Research Assistant
Biophysics and Chemical Physics

Department of Physics Sept. 89 - May 90
University of California, Berkeley, CA, USA
Teaching Assistant

Department of Physics Jan. 88 - May 88
University of California, Berkeley, CA, USA
Teaching Assistant

Department of Physics June 87 - Aug. 87
University of California, Berkeley, CA, USA
Research Assistant
Biophysics

Department of Physics Sept. 86 - May 87
University of California, Berkeley, CA, USA
Teaching Assistant

**Past Invited
Professorships**

Department of Chemistry
Duke University USA
Visiting Professor
Present, Aug.10 - Aug. 11, Jan. 08-July 11, June 05 - June 06, July 04 - Dec. 04

Department of Physics Sept. 04 - Dec. 04
Duke University USA
Visiting Professor

**Military
Service**

24/5/99-24/8/99 and 19/12/02-27/12/02

**Research
Funding**

FP7-PEOPLE-2012-IRSES "ELECTRONANOMAT": MOLECULAR SCALE ELECTROCHEMISTRY AND NONTRADITIONAL ELECTROCHEMICAL MATERIALS SCIENCE (2013-2016) (287700 EUR)
Collaborating institutions: Technical University of Denmark (DENMARK), University of Liverpool (UK), University of Alicante (SPAIN), Changchun Institute of Applied Chemistry, Chinese Academy of Science, Shanghai University, East China University of

Science and Technology (CHI)

COST ACTION "PERSPECT-H2O-SUPRAMOLECULAR PHOTOCATALYTIC WATER SPLITTING" CM1202 (2012-2016). Participated as expert (proposer: Professor B. Dietzek, Institute of Photonic Technology Jena, Germany)

VIBRATIONAL CONTROL OF ELECTRON TRANSFER (2011-2012),
Cyprus Research Promotion Foundation (100%) (60000 EUR).
Project coordinator. With Prof. D.N. Beratan (Duke Univ. USA)

CY-TERA A MULTI-TERAFLOP/s COMPUTING FACILITY FOR SCIENCE AND TECHNOLOGY
IN CYPRUS (2009-2013),
Cyprus Research Promotion Foundation (100%) (170000 EUR).
As a member of the project's University of Cyprus team.

STUDY OF THE MOLECULE COMPSTATIN, AN IMPORTANT INHIBITOR OF THE IMMUNE
SYSTEM, WITH HIGH PRECISION BIOMOLECULAR SIMULATIONS (2004-2007)
Funded by the Cyprus Research Promotion Foundation (75%) and the
University of Cyprus (25%)
Total funding: 40,000 CYP (69,600 EUR)
With Prof. G. Archontis (Univ. of Cyprus)

REPAIR OF UV-DAMAGED DNA BY DNA PHOTOLYASE: INSIGHTS FROM MOLECULAR
DYNAMICS SIMULATIONS AND ELECTRON TRANSFER CALCULATIONS (2003-2006)
Funded by the University of Cyprus
Total funding: 60,000 CYP (104,500 EUR)
With Prof. G. Archontis

REGULATION OF GLYCOGEN METABOLISM AND OXIDATIVE REPAIR OF DNA BY
MOLECULAR ASSOCIATION: INSIGHTS FROM SIMULATIONS AND EXPERIMENT (2002-2004)
Funded by the Leventis Foundation
Total funding: 37,000 CYP (64,400 EUR)
With Professors G. Archontis, and A. Nicolaides (Univ. of Cyprus)

FROM STRONG INTERACTIONS TO MOLECULAR RECOGNITION: THEORETICAL AND
COMPUTATIONAL STUDIES (1997-2000)
Funded by the University of Cyprus
Total funding: 160,000 CYP (280,000 EUR)
With Prof. Archontis for biophysics component
QCD component: Profs. C. Alexandrou and H. Panagopoulos (Univ. of Cyprus)

Under review

COST ACTION: "LIGHT INDUCED ACTION IN MACROMOLECULES AND MOLECULAR MATERIALS:
FROM SIMULATING THE INFLUENCE OF THE ENVIRONMENT TO TARGET- SPECIFIC CONTROL
(LIF: CONTROL OF LIGHT-INDUCED FUNCTIONS). Cyprus participant

**International
Collaborations**

Prof. David Beratan (Duke Univ. USA), Prof. David Cahen (Weizmann Institute, Israel),
Prof. Qijin Chi (DTU Denmark), Prof. Juan Carlos Cuevas (UAM, Spain), Prof. M.

(past & present) Elstner (KIT Germany), Prof. Wenbin Lin (UNC Chapel Hill, USA), Prof. Thomas Meyer (UNC Chapel Hill, USA), Prof. Ron Naaman (Weizmann Institute, Israel), Prof. Abraham Nitzan (Tel-Aviv Univ., Israel), Prof. John Papanikolas (UNC Chapel Hill, USA), Prof. Danny Porath (Hebrew Univ., Israel), Prof. Igor V. Rubtsov (Tulane University, USA), Prof. Jonathan L. Sessler (Univ. of Texas at Austin), Prof. Jens Ulstrup (DTU Denmark), Prof. David H. Waldeck (University of Pittsburgh, USA) Prof. Wei Yan (SHU, China), Profs. Chongjun Zao (ECUST, China)

**Conference/
School
Organization**

BIOELECTRONICS: PRINCIPLES, MATERIALS AND PROPERTIES
International School of Solid State Physics 60th Course
Ettore Majorana Foundation and Centre for Scientific Culture,
Erice, Sicily, Italy, April 30 – May 9, 2014
Organizing Committee:
D. N. Beratan (Duke Univ.), D. Cahen (Weizmann Inst.), P. Facci (CNR-IBF) & S. S. Skourtis (Univ. of Cyprus)
VILLA CONFERENCE ON INTERACTIONS BETWEEN NANOSTRUCTURES
Rocabella Resorts & Spa Hotel, Santorini Greece, June 21 - 25 2010
Member of International Organizing Committee

ELECTRONIC AND MAGNETIC PROPERTIES OF CHIRAL STRUCTURES AND THEIR ASSEMBLIES
Telluride Science Research Center, Telluride, CO USA,
July 26 - July 30, 2012
June 28 - July 2, 2010
Organizing Committee:
R. Naaman (Weizmann Inst.), D. N. Beratan (Duke Univ.), S. S. Skourtis (Univ. of Cyprus) & D. Waldeck (Univ. of Pittsburgh)

VILLA CONFERENCE ON INTERACTIONS BETWEEN NANOSTRUCTURES
Rocabella Resorts & Spa Hotel, Santorini Greece, June 21 - 25 2010
Member of International Organizing Committee

2nd SESAME WORKSHOP ON STRUCTURAL MOLECULAR BIOLOGY (SMB)
(Synchrotron Light for Experimental Science and Applications in the Middle East) Nicosia Cyprus, Dec 6 - 7, 2000
Organizing Committee:
G. Archontis & S. S. Skourtis (Univ. of Cyprus)
A. Perrakis (EMBL)
P. Kuhn (SSRL/Stanford Univ.)
E. Alp (Cochair, SESAME Sci. Comm. & APS/Argonne)
H. Winick (Cochair, SESAME Sci. Comm & SSRL/Stanford Univ.)

Publications

Total number of citations: 1137 (Skourtis SS, ISI 14/11/2013, h-index:21)

Jiaying Lin, Xiangqian Hu, Peng Zhang, et. al.
Triplet Excitation Energy Dynamics in Metal-Organic Frameworks
J. Phys. Chem. C. 117, 22250-22259 (2013)

Spiros S. Skourtis
Protein electron transfer

in Quantum Effects in Biology Cambridge University Press (invited book chapter)
M. Mohseni, Y. Omar, G. Engel, and M.B. Plenio, editors, In Press

Spiros S. Skourtis

Probing electron transfer mechanism from the molecular to the cellular length scales
Special issue on "Peptide-mediated electron and energy transport" (invited article)
Biopolymers (Peptide Science) 100, 82-92 (2012)

D. N. Beratan and S.S. Skourtis Electron transfer through proteins Encyclopedia of Biophysics G.C.K. Roberts (ed.), Springer-Verlag Berlin Heidelberg (2012).

Aleksey E. Kuznetsov, Balamurugan Desinghu, Spiros S. Skourtis, David N. Beratan
Structural and Electronic Properties of Bare and Capped Cd_nSe_n/Cd_nTe_n
Nanoparticles ($n = 6, 9$)
J. Phys. Chem. C 116, 6817–6830 (2012)

David N. Beratan and Spiros S. Skourtis
Electron transfer through proteins
Encyclopedia of Biophysics G.C.K. Roberts (ed.),
Springer-Verlag Berlin Heidelberg (2012).

Nicholas Polizzi, Spiros S. Skourtis, David N. Beratan
Physical constraints on charge transport through bacterial nanowires
Faraday Discussions 155, 43-62 (2012)

Spiros S. Skourtis, David N. Beratan and David H. Waldeck
Coherence in electron transfer pathways
In Proceedings of the 22nd Solvay Conference in Chemistry
"Quantum Effects in Chemistry and Biology"
Procedia Chemistry 3 99-104 (2011)

Horacio Carias, David N. Beratan and Spiros S. Skourtis
Floquet Analysis for Vibronically Modulated Electron Tunneling
J. Phys. Chem. B 115, 5510-5518 (2011)

Vered Ben-Moshe, David N. Beratan, Abraham Nitzan, and Spiros S. Skourtis
Chiral control of current transfer in molecules
Topics in Curr. Chem. Vol. 298 259–278 (2011) Springer-Verlag Berlin Heidelberg

Spiros S. Skourtis, David H. Waldeck, and David N. Beratan
Fluctuations in biological and bioinspired electron-transfer reactions
Ann. Rev. Phys. Chem. Vol. 61 461-485 (2010)

Vered Ben Moshe, Durhba Rai, Spiros S. Skourtis, and Abraham Nitzan
Steady-state current transfer and scattering theory
J. Chem. Phys. 133, 054105 (2010)

Vered Ben Moshe, Abraham Nitzan, Spiros S. Skourtis, and David Beratan
Steady state theory of current transfer
J. Phys. Chem. C 114, 8005-8013 (2010)

Zhiwei Lin, Candace M. Lawrence, Dequan Xiao, Victor V. Kireev, Spiros S.

Skourtis, Jonathan L. Sessler, David N. Beratan and Igor V. Rubtsov
Modulating unimolecular charge transfer by exciting bridge vibrations
J. Am. Chem. Soc. 131, 18060–18062 (2009)

Dequan Xiao, Spiros S. Skourtis, Igor V. Rubtsov, David N. Beratan.
Turning charge transfer on and off in a molecular interferometer with vibronic pathways
Nano Lett. 9:1818-23 (2009)

David N. Beratan, Spiros S. Skourtis, Ilya A. Balabin, Alexander Balaeff,
Shahar Keinan, Ravindra Venkatramani and Dequan Xiao
Steering electrons on moving pathways
Accounts of Chemical Research 42, 1669-1678 (2009)

Ilya Balabin, Spiros S. Skourtis, and David N. Beratan
Electron transfer: Chemical roles of water (Advanced Review)
Wiley Encyclopaedia of Chemical Biology
T.P. Begeley, Ed. John, Wiley & Sons (2009)

Spiros S. Skourtis, David N. Beratan, Ron Naaman, Abraham Nitzan, and David H.
Waldeck
Chiral control of electron transmission through molecules
Phys. Rev. Lett. 101, 283103 (2008)

Ilya A. Balabin, David N. Beratan, and Spiros S. Skourtis
The persistence of structure over fluctuations in biological electron transfer reactions
Phys. Rev. Lett. 101, 158102 (2008)

Phanourios. Tamamis, Spiros S. Skourtis, Dimitrios Morikis, John D. Lambris,
and Georgios Archontis.
Conformational analysis of compstatin analogues with molecular dynamics
simulations in explicit water
J. Molecular Graphics and Modelling 26, 571-580 (2007).

Spiros S. Skourtis and David N. Beratan.
Photosynthesis from the Protein's Perspective.
Science. 316, 703-704 (2007)

Tatiana Prytkova, David N. Beratan, and Spiros S. Skourtis
Photo-selected electron transfer pathways in DNA photolyase
Proc. Natl. Acad. Sci. USA 104, 802-807 (2007)

Antonios Teklos and Spiros S. Skourtis
Comparative study of perturbative methods for computing electron tunneling
matrix elements with a nonorthogonal basis set
J. Chem. Phys. 125, 244103 1-9 (2006)

Spiros S. Skourtis, Jianpin Lin, and David N. Beratan
The effects of bridge motion on electron transfer reactions mediated by tunneling
Modern methods for Theoretical Physical Chemistry of Biopolymers, E. B. Starikov,
S. Tanaka, and J. P. Lewis, editors, Elsevier, pp. 357-379 (2006)

Antonios Teklos and Spiros S. Skourtis

Electron transfer through time-dependent bridges: differences between Franck-Condon and Born-Oppenheimer breakdown
Chemical Physics 319, 52-68 (2005)
Special Issue: Molecular Charge Transfer in Condensed Media - From Physics and Chemistry to Biology and Nano-engineering

Spiros S. Skourtis, Ilya Balabin, Tsutomu Kawatsu and David N. Beratan
Protein dynamics and electron transfer: electronic decoherence and non-Condon effects.
Proc. Natl. Acad. Sci. (USA) 102, 3552-3557 (2005)

Spiros S. Skourtis, David H. Waldeck and David N. Beratan
Inelastic electron tunneling erases coupling pathway interferences.
Journal of Physical Chemistry B 108, 15511-15518 (2004)

Spiros S. Skourtis
Electron transfer through fluctuating bridges: Tunneling by virtual transitions that break the Born-Oppenheimer approximation
Chemical Physics Letters 372, 224-231 (2003)

Spiros Skourtis and Abraham Nitzan
Effects of initial state preparation on the distance dependence of electron transfer through molecular bridges and wires
Journal of Chemical Physics 119, 6271-6276 (2003)

Spiros S. Skourtis, Georgios Archontis and Qian Xie
Electron transfer through fluctuating bridges: On the validity of the superexchange mechanism and time-dependent tunneling matrix elements
Journal of Chemical Physics 115, 9444-9462 (2001)

Spiros S. Skourtis and David N. Beratan
Single- and multi-electron transfer processes
In Electron Transfer in Chemistry (5 vol. monograph), Vol. 1: Principles, Theories, Methods and Techniques, V. Balzani, P. Piotrowiak and M.A.J. Rodgers, editors, Wiley-VCH Press, Weinheim, pp. 109-125 (2001)

Qian Xie, Georgios Archontis and Spiros S. Skourtis
Protein electron transfer: A numerical study of tunneling through fluctuating bridges
Chemical Physics Letters 312, 237-246 (1999)

Spiros S. Skourtis and David N. Beratan
Theories of structure-function relationships for bridge-mediated electron transfer reactions
Advances in Chemical Physics, 106, 377-452 (1999)

David N. Beratan and Spiros S. Skourtis
Protein-mediated electron-transfer: pathways, orbital interactions, and contact maps
In Biological Electron-Transfer Chains: Genetics, Composition and Mode of operation, G. W. Canters and E. Vlijgenboom, editors, Kluwer Academic Publisher,

Dordrecht, The Netherlands, pp. 9-27 (1998)

David N. Beratan and Spiros S. Skourtis
Electron transfer mechanisms
Current Opinion in Chemical Biology 2, 235-243 (1998)

Spiros S. Skourtis and David N. Beratan
High and low resolution theories of protein electron transfer
Journal of Biological Inorganic Chemistry 2, 378-386 (1997)

Spiros S. Skourtis and David N. Beratan
Electron transfer contact maps
Journal of Physical Chemistry 101, 1215-1234 (1997)

José N. Onuchic, Steven M. Risser, Spiros S. Skourtis, David N. Beratan.
The Design of starburst dendrimer electron transfer systems
In Molecular Electronics, M. Ratner and J. Jortner, editors, Iupac Chemistry for
the 21st Century series, Blackwell Science, Oxford UK, pp. 369-379 (1997)

Satyam Priyadarshy, Spiros S. Skourtis, Steven M. Risser, David N. Beratan
Bridge-mediated electronic interactions: Differences between Hamiltonian and
Green function partitioning in a non-orthogonal basis
Journal of Chemical Physics 104, 9473-9481 (1996)

Spiros S. Skourtis, José N. Onuchic and David N. Beratan
A method to analyze multi-pathway effects in protein mediated donor-acceptor
coupling interactions
Inorganica Chimica Acta 234, 167-175 (1996)

Spiros S. Skourtis and Shaul Mukamel
Superexchange versus sequential long range electron transfer; density matrix
pathways in Liouville space
Chemical Physics 197, 367-387 (1995)

W.B. Curry, M.D. Grabe, J.V. Kurnikov, S.S. Skourtis, D.N. Beratan, J.J. Regan,
A.J.A. Aquino, P. Beroza, J.N. Onuchic
Pathways, pathway tubes, pathway docking and propagators in electron transfer
proteins
Journal of Bioenergetics and Biomembranes 27, 285-293 (1995)

Spiros S. Skourtis, Jeffrey J. Regan and José N. Onuchic
Electron transfer in proteins: a novel approach for the description of donor-
acceptor coupling
Journal of Physical Chemistry 98, 3379-3388 (1994)

Spiros S. Skourtis, David N. Beratan and José N. Onuchic
The two-state reduction for electron and hole transfer in bridge-mediated electron
transfer reactions
Chemical Physics 176, 501-520 (1993)

Spiros S. Skourtis and José N. Onuchic
Effective two-state systems in bridge-mediated electron transfer: A Green's
function analysis
Chemical Physics Letters 209, 171-177 (1993)

Spiros S. Skourtis, Antonio J. R. da Silva, William Bialek, and José N. Onuchic
A new look at the primary charge separation in bacterial photosynthesis
Journal of Physical Chemistry 96, 8034-8041 (1992)

Submitted

Alexander Heck, Paul Woiczikowski, Tomas Kubar et. al.
The importance of backbone tunneling for electron transfer in model peptides
J. Phys. Chem. B.

Yuqi Zhang, Chaoren Liu, Alexander Balaeff, Spiros S. Skourtis, David N. Beratan
A flickering resonance mechanism for biological electron transfer
Proc. Natl. Acad. Sci. (USA)

In preparation

Desinghu Balamurugan, David N. Beratan, and Spiros S. Skourtis
Strategies enabling two-electron transfer in molecules and nanosystems

Danny Porath, Juan Carlos Cuevas, Agostino Migliore et. al.
Long range charge transfer in G4 DNA molecules

Conference Proceedings

Spiros S. Skourtis, Tatiana Prytkova and David N. Beratan
Flavin charge transfer transitions assist DNA photolyase electron transfer.
American Institute of Physics (AIP) Conference Proceedings 963 (Volume 2B),
pp 674-677 (2007).

COMPUTATION IN MODERN SCIENCE AND ENGINEERING:
Proceedings of the International Conference on Computational Methods in
Science and Engineering 2007 (ICCMSE 2007): VOLUME 2, PART B

Spiros S. Skourtis and David N. Beratan
A molecular double slit paradigm
American Institute of Physics (AIP) Conference Proceedings 963 (Volume 2B),
pp 809-812 (2007).

COMPUTATION IN MODERN SCIENCE AND ENGINEERING:
Proceedings of the International Conference on Computational Methods in
Science and Engineering 2007 (ICCMSE 2007)

Spiros S. Skourtis
The effects of biomolecular dynamics on biological electron transport
Proceedings of the XXI Hellenic Conference of Solid State Physics and Materials Science
Nicosia, Cyprus, August 28-31 2005 (2007), pp. 78-80.

Editorials

Spiros S. Skourtis and David N. Beratan
Guest Editorial: Electron Transfer
Molecular Simulation 32, 675-676 (2006)
Special issue: Electron transfer

**Invited
Talks (2012-14)
Conference &
Departmental**

“The flickering resonance mechanism for DNA charge transport”

"Charge Transport in Organic Materials " CECAM Workshop
University of Bremen, Germany (31 March – 4 April 2014)

“Rare events in molecular and biomolecular electron transfer reactions”

Symposium on "Rare Events: optimal solutions and challenges - from charge transfer reactions to supervolcanoes" General Meeting of the German Physical Society
Humboldt University Berlin, Germany (19 March 2014)

“Physical Principles and Underlying Mechanisms of Biomolecules and Materials”

Institute of Physics, Chinese Academy of Sciences, Beijing, China (3-5 August 2013)
Biological electron transfer from the single-molecule to the cellular length scales: the roles of structure and fluctuations

Hebrew University Department of Chemistry Colloquium

Hebrew University, Jerusalem, Israel (11 April 2013)

Electron transfer and transport control: from small molecule to the cellular length scales

“Molecular Electronics in Jerusalem, International Meeting”

Institute of Advanced Studies, Hebrew University, Jerusalem, Israel (16-20 July 2012)
The control of electron and energy transfer pathways in small molecule and in biomolecular systems

“Quantum Effects in Biological Systems, QUEBS 2012” UC Berkeley (4-8 June 2012)

Electron transfer control: from small molecule to cellular length scales

Institute of NanoScience Italian National Research Council (CNRNano)

Center S3, Modena (May 24, 2012)

The control of electron and energy transfer pathways in molecular and cellular systems

*“Quantum Efficiency Colloquium” Institute of Physics, Albert Ludwigs University
Freiburg*

Freiburg, Germany (May 7-9, 2012)

“Quantum Malta 2012: Fundamental Problems in Quantum Physics”

University of Malta, Valetta Campus, Malta (April 24-27, 2012)

Biological electron transport processes

- Invited Conference Talks (2011)**
- “Quantum Coherence in Biology Symposium” American Physical Society Meeting*
Dallas Texas (March 21-25, 2011)
The control of electron transfer pathways in biomolecular systems: the role of fluctuations.
- “20 Years of Tunneling Pathways Symposium” American Chemical Society National Meeting*
Anaheim CA (March 27-31, 2011)
Control of electron transfer in biomolecular and small molecules systems:
Some open problems and connections with molecular devices
- “Solar Fuels: Light Capture and Electron Flow”*
European-US meeting of the COST Action D35, NSF CCI Solar and US Dept. of Energy JCAP projects
Prague, Czech Republic, (May 23-26, 2011).
Electron transfer pathway control in biomolecular and small molecule assemblies
- “Charge Transfer in Biosystems” ESF-LFUI conference. Universitätszentrum Obergurgl, Austria, (July 17-22, 2011).*
Ultrafast electron transfer in biological systems
- Invited Departmental Talks (2010-11)**
- Department of Biochemistry, Duke University USA* (Sept. 20 2010)
The quantum mechanics of biological electron transfer reactions
- Department of Physics, Duke University USA* (Sept. 30 2010)
Control of electron transport pathways in biomolecules and small molecule systems
- Department of Chemistry, UNC Chapel Hill USA* (Feb. 10, 2011)
The control of electron transfer pathways in biomolecular and small-molecule device systems: the roles of medium fluctuations and initial state preparation
- Department of Physics University of Miami, FLA USA* (April 13 2011)
The control of electron transfer pathways in biomolecular and small-molecule device systems: the roles of medium fluctuations and initial state preparation
- Other Recent Conference Presentations**
- Invited Talks*
- “Frontiers in Biophysics” Focus Session of the “6th International Discussion Meeting on Relaxations in Complex Systems”*
Rome, Italy (Aug. 30-Sept. 5, 2009)
Open problems in biological electron transfer processes and connections with molecular devices
- EPSRC Symposium Workshop on Quantum Simulations*
University of Warwick, UK (Aug. 24-28, 2009)
Biological and small molecule electron transfer processes: some interesting connections
- “Electron Transfer and Transmission – New aspects”, Mini-Symposium*

The Weizmann Institute, Rehovot, Israel, (May 25, 2009)
Double-slit electron transfer molecular devices and other interesting systems

Duke University “Adventures in Theory Lecture Series”

Duke Univ. USA (Aug. 13 2008)
Electron transport in fluctuating biological media

1st meeting of the Hellenic group of biological physics.

National Hellenic Foundation. Athens Greece (Nov. 3, 2007)
Biological electron transport mechanisms: From tunneling to thermally activated hopping

International Conference of Computational Methods in Sciences and Engineering 2007

Corfu, Greece, (Sept 25-30)
A molecular double slit paradigm.
"Quantum Control and Light-Matter Interactions: Recent Computational and Theoretical Results" symposium.
Flavin charge transfer transitions assist DNA photolyase electron transfer.
"Modeling Complex Molecular and Biomaterial Systems" symposium.

Contributed Talks

“Science for Our Nation’s Energy Future: Energy Frontier Research Centers Summit & Forum”

DOE, Washington DC, USA, May 26-27 2011
Session: Solar Fuels and Next Generation Photovoltaics
WenBin Lin & S.S. Skourtis
Framework materials for solar energy applications

“Radiation Damage in Biomolecular Systems (RADAM) 2008”

Debrecen, Hungary (June 13-15 2008)
The role of flavin charge transfer transitions in biological electron transfer reactions: the case of DNA photolyase

“XXI Panhellenic Conference of Solid State Physics and Materials Science”

Nicosia Cyprus (28-30 Aug. , 2005)
The effects of biomolecular dynamics on biological electron transport

Other Conference Participation

“2nd SESAME Workshop on Structural Molecular Biology (SMB)”

Nicosia, Cyprus, (6-7 Dec, 2000)
Co-organizer

“3rd Meeting of the International Interim Council of SESAME (UNESCO)”

Amman, Jordan (June 20-21, 2000)
Representative of Cyprus

“1st SESAME Workshop on Structural Molecular Biology (SMB)”

Athens, Greece (6-7 April, 2000)

(SESAME: Synchrotron Light for Experimental Science and Applications in the Middle East)

College on Methods and Experimental Techniques in Biophysics
International Center for Theoretical Physics, Trieste, Italy, (Sept.28- Oct. 23, 1999)

**Research
Supervision**

Department of Physics University of Cyprus

Graduate student: Panayiotis Antoniou 2009-present
Masters and Ph.D. thesis advising

Undergraduate students Aristi Christofi and Michalis Panagiotou 2006 – 07, 07-08
Undergraduate fourth-year thesis
Undergraduate thesis research involves modeling electron transfer reactions in Cryptochromes and DNA photolyases.

Undergraduate student Antonios Teklos 2001 - 02
Undergraduate fourth-year thesis
Thesis title: Effective Hamiltonians for time-dependent tight-binding systems
Published one article on the subject.

Graduate student Antonios Teklos 2002 - 05
Masters thesis advising
Thesis subject: Effects of basis set nonorthogonality on Green's function calculations for electron transfer reactions.
Published one article on the subject.

Post-doctoral fellow Dr. Qian Xie 1997 - 2000
Research funded under the program:
"From Strong Interactions to Molecular Recognition: Theoretical and Computational studies"
Published two articles on electron transfer theory

Post-doctoral fellow Dr. Majid Monajjemi Feb. 03 - Sept. 03
Research funded under the program:
"Regulation of Glycogen metabolism and oxidative repair of DNA by molecular association; Insights from simulations and experiment"

Post-doctoral fellow Dr. Haidar Sabbagh Nov. 03 - March 04
Research funded under the program:
"Repair of UV-damaged DNA by DNA photolyase; Insights from molecular simulations and electron transfer calculations"

Department of Chemistry, University of Pittsburgh, PA, USA

Undergraduate intern Michael Grabe Summer 95, 96

Research on protein electron transfer
Main student advisor: Prof. D.N. Beratan

Department of Chemistry, Duke University, NC, USA

Ph.D. student Dequan Xiao 2006-2008
Research on electron transfer in molecular electronic devices
I was an external member of D. Xiao's Ph.D. committee and co-author in submitted paper

Department of Physics, Duke University, NC, USA

Ph.D. student Horacio Carias 2008-2011
Research on electron transfer in molecular electronic devices
External member of Mr. Carias' Ph.D. committee and co-supervisor in his Ph.D thesis

Ph.D. student Nan Jiang 2010-present
Research on electron transfer reactions in cryptochromes
Co-supervisor in Ph.D thesis

Teaching

Department of Physics University of Cyprus

Quantum Mechanics of Biomolecular Systems
(Theoretical and Computational Methods)
Second year, one-semester course for physics graduates (Masters, Ph.D)
An introduction to the quantum mechanics of open systems (quantum master equations), and to molecular electronic structure, with applications to chemical and biological electron transfer

Textbooks:

- (1) A. Nitzan, *Chemical Dynamics in Condensed Phases: Relaxation, Transfer, and Reactions in Condensed Molecular Systems*, Oxford (2006).
- (2) A.M. Kuznetsov and J. Ulstrup, *Electron Transfer in Chemistry and Biology*, Wiley, Chichester (1999)
- (3) V. May and O. Kuhn, *Charge and Energy Transfer Dynamics in Molecular Systems: A Theoretical Introduction*, John Wiley (2000)

Computational Physics

Fourth year, one-semester course for physics undergraduates:
Ordinary differential equations, computational linear algebra, data analysis, partial differential equations, stochastic methods, selected applications from classical mechanics, electrodynamics, statistical mechanics and quantum mechanics.

Main textbooks:

- (1) A. L. Garcia, *Numerical Methods for Physics*, Prentice Hall, (2nd edition)
- (2) H. Gould and J. Tobochnik. *An introduction to Computer Simulation Methods*, Addison Wesley, (2nd edition)

- (3) P.L. DeVries, J.E. Hasbun *A First Course in Computational Physics*, Jones & Bartlett Publishers, (2nd edition)
(4) T. Pang *An Introduction to Computational Physics* Cambridge University Press, (2nd edition)

Atomic and Molecular Physics

Fourth year, one-semester course for physics undergraduates:

The hydrogen atom, angular momentum/spin and addition of angular momenta, the Stark, Zeeman and spin-orbit effects, the Born-Oppenheimer approximation, the theory of the chemical bond (H_2^+ , H_2 , valence-bond and molecular orbital theories), and molecular electronic structure.

Main textbook:

P. W. Atkins, *Molecular Quantum Mechanics*, Oxford University Press (1986) (2nd edition)

Quantum Mechanics (I)

Fourth semester course for physics undergraduates:

The Schrödinger equation (one dimensional problems with bound and scattering states, and the hydrogen atom), the Hilbert space formalism, the generalized statistical interpretation, angular momentum, and spin.

Main textbook:

D. J. Griffiths, *Introduction to Quantum Mechanics*, Prentice Hall (1995)

Electromagnetism (I)

Fourth semester course for physics undergraduates:

Vector calculus, electrostatics, general methods for Laplace's equation, electric fields in matter, magnetostatics, magnetic fields in matter, electrodynamics (electromotive force, electromagnetic induction, Maxwell's equations).

Main textbook:

D. J. Griffiths, *Introduction to Electrodynamics*, Pearson (2013)

Physics and Applications

General service course for non-physics undergraduates:

I discuss important concepts and results of classical and quantum mechanics at an introductory level. The emphasis is on comparisons between the classical and quantum dynamics of simple systems (e.g., the free particle, the harmonic oscillator, and rotational motion). Several introductory textbooks were used.

Department of Physics & INFN-S3 University of Modena, Modena, Italy

PhD School on Physics and Nano Sciences

Ph.D short course

May 21-24 2012

Electron transfer pathway control in biomolecular and small molecule systems:
the role of fluctuations (used personal notes)

Department of Physics, University of California, San Diego, USA

Graduate biophysics seminar Spring 92
I taught path-integral techniques

Books used:

- (1) A. Ranfagni, D. Mugnai, P. Morreti, M. Cetica, *Trajectories and Rays: The Path Summation in Quantum Mechanics and Optics - Vol. I*, World Scientific (1990)
- (2) J. W. Negele, H. Orland, *Quantum Many-Particle Systems*, Addison Wesley (1988)

Department of Physics, University of California, Berkeley, USA

Teaching Assistant (laboratory, discussion and grading). Courses taught:

Introductory physics (I) Spring 87, Fall 89, Spring 90
Mechanics, Wave motion, Electrostatics and Heat

Descriptive introductory physics Spring 88
A brief presentation of some of the more important phenomena in physics with experimental illustration

Physics for scientists and engineers (II) Fall 86
Electricity and Magnetism

**Administrative
And Other
Activities**

Science representative of Cyprus
Interim Council for the SESAME project (UNESCO) 2000-01
Participated in the 3rd Meeting of the Interim Council of the SESAME Project (June 21-22 2000, Amman, Jordan). Cyprus was a member country of the SESAME project (Synchrotron-light for Experimental Science and Applications in the Middle East).

University of Cyprus
Departmental physics seminars organizer Fall 97 - Spring 03
Seminars involved international speakers

Computer Systems Evaluation Committee Aug. 97 - Nov. 97
The committee evaluated and compared the performance of all PC and server models reviewed by the university for purchase in 1998

Department of Physics Chairperson, Feb. 08 – Feb. 10
Department of Physics, University of Cyprus

Member of the Academic Council of the School of Pure and Applied Sciences, Feb. 08 – Feb. 10
University of Cyprus

Member of the Ad Hoc Graduate Faculty Aug. 08 – July 10
Duke University

(Member of Ph.D. committee of Chemistry Dept. graduate student Dequan Xiao)

Member of Resource Allocation Committee (current)
Computation-based Science and Technology Research Center (CaSToRC)
Cyprus Institute

Other recurrent duties

Served in the departmental board that evaluates visiting teaching-professor applications, and in a cross-departmental working group for the creation of inter-disciplinary studies. Member of the departmental committee for the Ph.D. entrance examinations, and for physics teaching for high-school students. Member of the university committee that develops policy for students with disabilities and special needs.

Manuscript Refereeing	Journals: Chemical Physics, Chemical Physics Letters, Journal of the American Chemical Society, Journal of Chemical Physics, Journals of Physical Chemistry, Nanotechnology, Nature Nanotechnology, Proc. Natl. Acad. Sci. USA, New Journal of Physics.
Agency Refereeing	Israel Science Foundation National Science Foundation (USA)
Journal Editing	Guest co-editor (with Prof. D. N. Beratan) <u>Molecular Simulation</u> Vol 32, Number 9, August 2006 Special issue: Electron transfer Associate Editor (March 2011-14) <u>BMC Biophysics</u> BioMed Central
Languages	Greek, English, Spanish